

10500319

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TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	JAN 17	Pre-1988 INPI data added to MARPAT
NEWS 4	FEB 21	STN AnaVist, Version 1.1, lets you share your STN AnaVist visualization results
NEWS 5	FEB 22	The IPC thesaurus added to additional patent databases on STN
NEWS 6	FEB 22	Updates in EPFULL; IPC 8 enhancements added
NEWS 7	FEB 27	New STN AnaVist pricing effective March 1, 2006
NEWS 8	MAR 03	Updates in PATDPA; addition of IPC 8 data without attributes
NEWS 9	MAR 22	EMBASE is now updated on a daily basis
NEWS 10	APR 03	New IPC 8 fields and IPC thesaurus added to PATDPAFULL
NEWS 11	APR 03	Bibliographic data updates resume; new IPC 8 fields and IPC thesaurus added in PCTFULL
NEWS 12	APR 04	STN AnaVist \$500 visualization usage credit offered
NEWS 13	APR 12	LINSPEC, learning database for INSPEC, reloaded and enhanced
NEWS 14	APR 12	Improved structure highlighting in FQHIT and QHIT display in MARPAT
NEWS 15	APR 12	Derwent World Patents Index to be reloaded and enhanced during second quarter; strategies may be affected
NEWS 16	MAY 10	CA/CAPLUS enhanced with 1900-1906 U.S. patent records
NEWS 17	MAY 11	KOREAPAT updates resume
NEWS 18	MAY 19	Derwent World Patents Index to be reloaded and enhanced
NEWS 19	MAY 30	IPC 8 Rolled-up Core codes added to CA/CAPLUS and USPATFULL/USPAT2
NEWS 20	MAY 30	The F-Term thesaurus is now available in CA/CAPLUS
NEWS 21	JUN 02	The first reclassification of IPC codes now complete in INPADOC
NEWS EXPRESS		FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005. V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT http://download.cas.org/express/v8.0-Discover/
NEWS HOURS		STN Operating Hours Plus Help Desk Availability
NEWS LOGIN		Welcome Banner and News Items
NEWS IPC8		For general information regarding STN implementation of IPC 8
NEWS X25		X.25 communication option no longer available after June 2006

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 11:15:52 ON 08 JUN 2006

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 11:16:04 ON 08 JUN 2006

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STRUCTURE FILE UPDATES: 7 JUN 2006 HIGHEST RN 887123-67-3

DICTIONARY FILE UPDATES: 7 JUN 2006 HIGHEST RN 887123-67-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

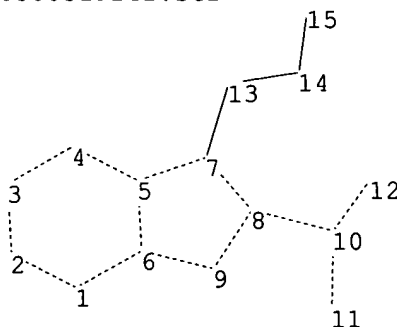
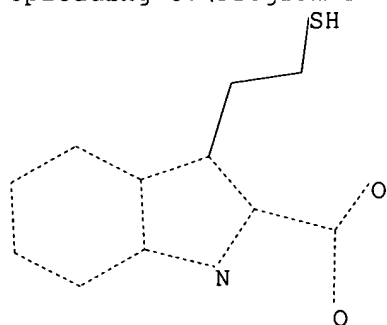
Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10500319rtr.str



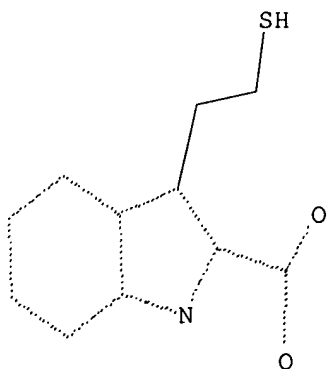
10500319

chain nodes :
10 11 12 13 14 15
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
7-13 8-10 10-11 10-12 13-14 14-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 8-10 10-11 10-12 14-15
exact bonds :
7-13 13-14

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS

L1 STRUCTURE UPLOADED

=> d 11
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11
SAMPLE SEARCH INITIATED 11:16:27 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 314 TO ITERATE

100.0% PROCESSED 314 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 5217 TO 7343
PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> s 11 full
FULL SEARCH INITIATED 11:16:34 FILE 'REGISTRY'

10500319

FULL SCREEN SEARCH COMPLETED - 5497 TO ITERATE

100.0% PROCESSED 5497 ITERATIONS 14 ANSWERS
SEARCH TIME: 00.00.01

L3 14 SEA SSS FUL L1

=> fil hcaplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

166.94

167.15

FILE 'HCAPLUS' ENTERED AT 11:16:39 ON 08 JUN 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 8 Jun 2006 VOL 144 ISS 24
FILE LAST UPDATED: 7 Jun 2006 (20060607/ED)

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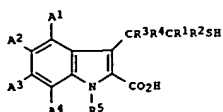
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3

L4 1 L3

=> d ed abs ibib hitstr

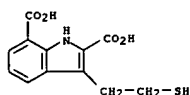
L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 18 Jul 2003
GI



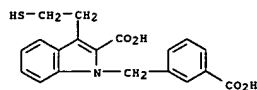
AB This invention relates to new indoles (shown as I; variables defined below: e.g. 3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid), pharmaceutical compns. and diagnostic kits comprising such compds., and methods of using such compds. for inhibiting NAALADase enzyme activity, detecting diseases where NAALADase levels are altered, affecting neuronal activity, effecting TGF- β activity, inhibiting angiogenesis, and treating glutamate abnormalities, neuropathy, pain, compulsive disorders, prostate diseases, cancers and glaucoma. IC50 values are tabulated for inhibition of NAALADase by 12 examples of I. Many pharmacol. and therapeutic test results are reported for the following 6 compds. that are not covered by I: 2-[(2,3,4,5,6-pentafluorobenzyl)hydroxyphosphinyl]methyl pentanedioic acid, 2-(3-sulfanylpentyl)pentanedioic acid, 2-(phosphonomethyl)pentanedioic acid, 2-(2-sulfanylpentyl)pentanedioic acid, 3-carboxy- α -(3-mercaptopropyl)benzenepropanoic acid and 3-carboxy-5-(1,1-dimethylethyl)- α -(3-mercaptopropyl)benzenepropanoic acid. For I: A1, A2, A3 and A4 = H, C1-C9 alkyl, C2-C9 alkenyl, C2-C9 alkynyl, aryl, heteroaryl, carbocycle, heterocycle, C1-C9 alkoxy, C2-C9 alkenyloxy, phenoxy, benzyloxy, hydroxy, halo, nitro, cyano, isocyano, -COOR6, -COR6, -NR6R7, -SR6, -SOR6, -SO2R6, -SO2(OR6), -C(O)NR6R7, -C(O)NR6 (CH2)nCOOH, -NR6C(O)R7 or -(CH2)nCOOH, or any adjacent two of A1, A2, A3 and A4 form with the benzene ring a fused ring that is (un)saturated, aromatic or nonarom., and carbocyclic or heterocyclic, said heterocyclic ring containing 1 or 2 O, N and/or S heteroatom(s); n is 1-3; R, R1, R2, R3, R4, R5, R6, R7 = H, carboxy, C1-C9 alkyl, C2-C9 alkenyl, C2-C9 alkynyl, aryl, heteroaryl, carbocycle or heterocycle; and said alkyl, alkenyl, alkynyl, aryl, heteroaryl, carbocycle, heterocycle, alkoxy, alkenyloxy, phenoxy, benzyloxy and fused ring (un)substituted with ≥ 1 substituent(s). Although the methods of preparation are not claimed, 13 example preps. are included.

ACCESSION NUMBER: 2003:551494 HCAPLUS
DOCUMENT NUMBER: 139:101027
TITLE: Preparation of mercaptoethyl indolecarboxylic acids as NAALADase inhibitors for treating and diagnosing glutamate abnormalities, neurological and other disorders
INVENTOR(S): Tsukamoto, Takashi; Grella, Brian; Majer, Pavel
PATENT ASSIGNEE(S): Guilford Pharmaceuticals Inc., USA
SOURCE: PCT Int. Appl., 173 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

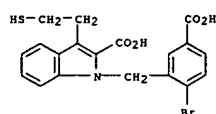
L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 560131-42-2 HCAPLUS
CN 1H-Indole-2,7-dicarboxylic acid, 3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)



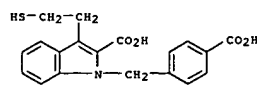
RN 560131-44-4 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 1-[(3-carboxyphenyl)methyl]-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)



RN 560131-46-6 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 1-[(2-bromo-5-carboxyphenyl)methyl]-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)



RN 560131-47-7 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 1-[(4-carboxyphenyl)methyl]-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)



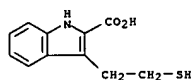
RN 560131-48-8 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 3-(2-mercaptoethyl)-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

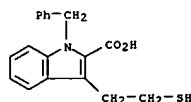
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003057670	A2	20030717	WO 2002-US37617	20021219
WO 2003057670	A3	20031106		
V: AZ, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, EC, EE, ES, FI, GB, GD, GE, GR, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TH, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GN, GW, GU, GY, HT, HR, KE, KM, MT, MU, NI, NG, NO, NP, PA, PG, PH, PY, RE, RW, SC, SD, SE, SG, SH, SI, SL, SM, SN, ST, SV, TD, TG, TN, TZ, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
AU 2002357003	A1	20030724	AU 2002-357003	20021219
US 2005080128	A1	20050414	US 2003-500319	20021219
PRIORITY APPLN. INFO.: US 2001-342764P P 20011228 WO 2002-US37617 W 20021219				

OTHER SOURCE(S): MARPAT 139:101027
IT 560131-39-7P, 3-(2-Mercaptoethyl)-1H-indole-2-carboxylic acid
560131-42-2P, 3-(2-Mercaptoethyl)-1H-indole-2,7-dicarboxylic acid
560131-44-4P, 1-[(3-Carboxyphenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-46-6P, 1-[(2-Bromo-5-carboxyphenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-47-7P, 1-[(4-Carboxyphenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-48-8P, 3-(2-Mercaptoethyl)-1-(phenylmethyl)-1H-indole-2-carboxylic acid 560131-49-9P, 1-[(2-Carboxyphenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-50-2P, 1-[(3-Carboxy-5-(1,1-dimethylethyl)phenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-51-3P, 1-[(4-Bromo-3-carboxyphenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-52-4P, 1-[(2-Carboxy-5-methoxyphenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-53-5P, 3-(2-Mercaptoethyl)-1-(2-phenylethyl)-1H-indole-2-carboxylic acid 560131-54-6P, 3-(2-Mercaptoethyl)-1-phenyl-1H-indole-2-carboxylic acid 560131-56-8P, 1-(3-Carboxyphenyl)-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-65-9P, 1-(3-Carboxy-5-(1,1-dimethylethyl)phenyl)-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid
RL: DGM (Diagnostic use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USGS (Uses)
(drug candidate and diagnosis agent; preparation of mercaptoethyl indolecarboxylic acids as NAALADase inhibitors for treating and diagnosing glutamate abnormalities and neurol. and other disorders)

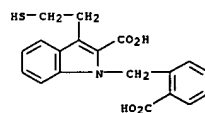
RN 560131-39-7 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)



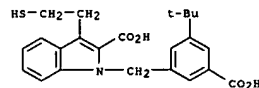
L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



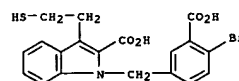
RN 560131-49-9 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 1-[(2-carboxyphenyl)methyl]-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)



RN 560131-50-2 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 1-[(3-carboxy-5-(1,1-dimethylethyl)phenyl)methyl]-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)



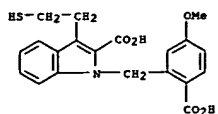
RN 560131-51-3 HCAPLUS
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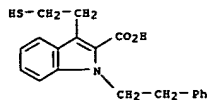
RN 560131-52-4 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 1-[(2-carboxy-5-methoxyphenyl)methyl]-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)

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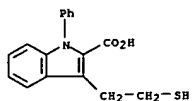
L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



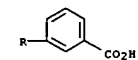
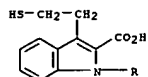
RN 560131-53-5 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 3-(2-mercaptoethyl)-1-(2-phenylethyl)- (9CI) (CA INDEX NAME)



RN 560131-54-6 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 3-(2-mercaptoethyl)-1-phenyl- (9CI) (CA INDEX NAME)

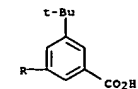
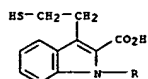


RN 560131-56-8 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 1-(3-carboxyphenyl)-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 560131-65-9 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 1-(3-carboxy-5-(1,1-dimethylethyl)phenyl)-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)



10500319

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

7.64

174.79

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-0.75

-0.75

FILE 'REGISTRY' ENTERED AT 11:17:06 ON 08 JUN 2006

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 7 JUN 2006 HIGHEST RN 887123-67-3

DICTIONARY FILE UPDATES: 7 JUN 2006 HIGHEST RN 887123-67-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

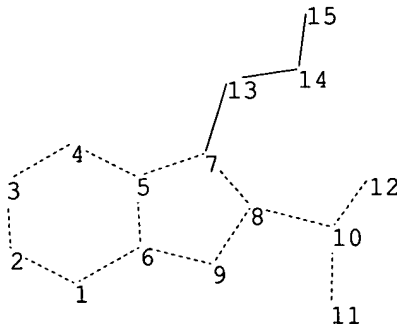
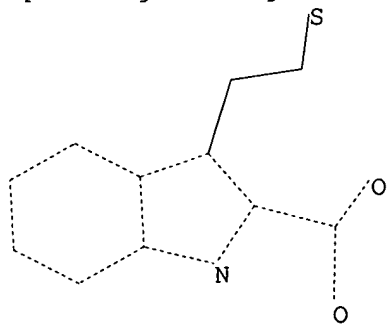
Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10500319s2.str



chain nodes :

10500319

10 11 12 13 14 15

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

7-13 8-10 10-11 10-12 13-14 14-15

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 8-10 10-11 10-12 14-15

exact bonds :

7-13 13-14

Match level :

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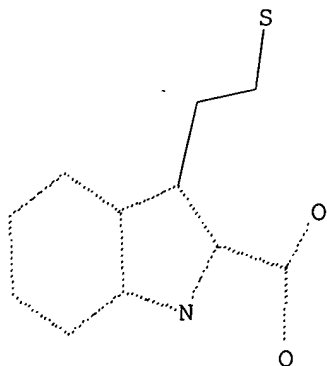
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS

L5 STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS

L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 15

SAMPLE SEARCH INITIATED 11:18:42 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 314 TO ITERATE

100.0% PROCESSED 314 ITERATIONS

3 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 5217 TO 7343

PROJECTED ANSWERS: 3 TO 163

L6 3 SEA SSS SAM L5

=> s 15 full

FULL SEARCH INITIATED 11:18:47 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 5497 TO ITERATE

10500319

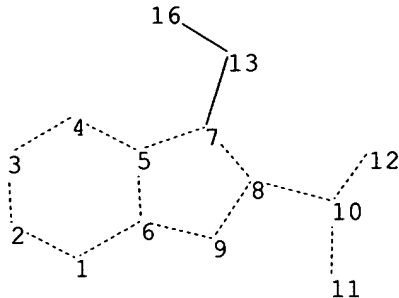
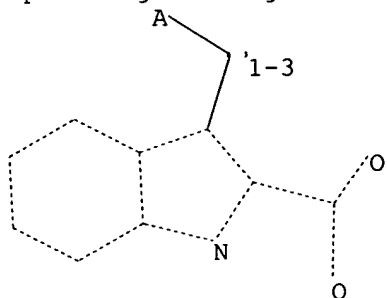
100.0% PROCESSED 5497 ITERATIONS
SEARCH TIME: 00.00.01

21 ANSWERS

L7 21 SEA SSS FUL L5

=>

Uploading C:\Program Files\Stnexp\Queries\10500319s3.str



chain nodes :

10 11 12 13 16

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

7-13 8-10 10-11 10-12 13-16

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 8-10 10-11 10-12 13-16

exact bonds :

7-13

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

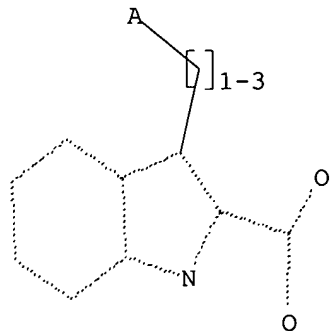
11:CLASS 12:CLASS 13:CLASS 16:CLASS

L8 STRUCTURE UPLOADED

=> d 18

L8 HAS NO ANSWERS

L8 STR



Structure attributes must be viewed using STN Express query preparation.

10500319

=> s l8

SAMPLE SEARCH INITIATED 11:21:33 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5004 TO ITERATE

40.0% PROCESSED 2000 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 95839 TO 104321
PROJECTED ANSWERS: 3110 TO 4796

L9 50 SEA SSS SAM L8

=> s l8 full

FULL SEARCH INITIATED 11:21:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 99151 TO ITERATE

100.0% PROCESSED 99151 ITERATIONS 3611 ANSWERS
SEARCH TIME: 00.00.01

L10 3611 SEA SSS FUL L8

=> fil hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	336.52	511.31
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.75

FILE 'HCAPLUS' ENTERED AT 11:21:45 ON 08 JUN 2006
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FILE COVERS 1907 - 8 Jun 2006 VOL 144 ISS 24
FILE LAST UPDATED: 7 Jun 2006 (20060607/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 11:15:52 ON 08 JUN 2006)

10500319

FILE 'REGISTRY' ENTERED AT 11:16:04 ON 08 JUN 2006
L1 STRUCTURE UPLOADED
L2 2 S L1
L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 11:16:39 ON 08 JUN 2006
L4 1 S L3

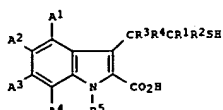
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L5 STRUCTURE UPLOADED
L6 3 S L5
L7 21 S L5 FULL
L8 STRUCTURE UPLOADED
L9 50 S L8
L10 3611 S L8 FULL

FILE 'HCAPLUS' ENTERED AT 11:21:45 ON 08 JUN 2006

=> s 17
L11 2 L7

=> d ed abs ibib hitstr 1-2

L11 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 18 Jul 2003
GI

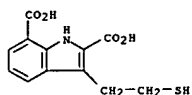


I

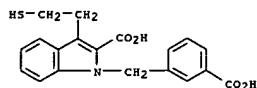
AB This invention relates to new indoles (shown as I; variables defined below: e.g. 3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid), pharmaceutical compns. and diagnostic kits comprising such compds., and methods of using such compds. for inhibiting NAALADase enzyme activity, detecting diseases where NAALADase levels are altered, affecting neuronal activity, effecting TGF- β activity, inhibiting angiogenesis, and treating glutamate abnormalities, neuropathy, pain, compulsive disorders, prostate diseases, cancers and glaucoma. IC50 values are tabulated for inhibition of NAALADase by 12 examples of I. Many pharmacol. and therapeutic test results are reported for the following 6 compds. that are not covered by I: 2-[[[(2,3,4,5,6-pentafluorobenzyl)hydroxyphosphinyl)methyl]pentanedioic acid, 2-(3-sulfanylpentyl)pentanedioic acid, 2-(phosphonomethyl)pentanedioic acid, 2-(2-sulfanylethyl)pentanedioic acid, 3-carboxy- α -(3-mercaptopropyl)benzenepropanoic acid and 3-carboxy-5-(1,1-dimethylethyl)- α -(3-mercaptopropyl)benzenepropanoic acid. For I: A1, A2, A3 and A4 = H, C1-C9 alkyl, C2-C9 alkenyl, C2-C9 alkynyl, aryl, heteroaryl, carbocyclic, heterocyclic, C1-C9 alkoxy, C2-C9 alkenyloxy, phenoxy, benzyloxy, hydroxy, halo, nitro, cyano, isocyanato, -COOR6, -COR6, -NR6R7, -SR6, -SOR6, -SO2R6, -SO2(OR6), -C(O)NR6R7, -C(O)NR6 (CH2)nCOOH, -NR6C(O)R7 or -(CH2)nCOOH, or any adjacent two of A1, A2, A3 and A4 form with the benzene ring a fused ring that is (un)saturated, aromatic or nonarom., and carbocyclic or heterocyclic, said heterocyclic ring containing 1 or 2 O, N and/or S heteroatom(s); n is 1-3; R, R1, R2, R3, R4, R5, R6, R7 = H, carboxy, C1-C9 alkyl, C2-C9 alkenyl, C2-C9 alkynyl, aryl, heteroaryl, carbocycle or heterocycle; and said alkyl, alkenyl, alkynyl, aryl, heteroaryl, carbocycle, heterocycle, alkoxy, alkenyloxy, phenoxy, benzyloxy and fused ring (un)substituted with ≥ 1 substituent(s). Although the methods of preparation are not claimed, 13 example preps. are included.

ACCESSION NUMBER: 2003:551494 HCAPLUS
DOCUMENT NUMBER: 139:101027
TITLE: Preparation of mercaptoethyl indolecarboxylic acids as NAALADase inhibitors for treating and diagnosing glutamate abnormalities, neurological and other disorders
INVENTOR(S): Tsukamoto, Takashi; Grella, Brian; Majer, Pavel
PATENT ASSIGNEE(S): Guilford Pharmaceuticals Inc., USA
SOURCE: PCT Int. Appl., 173 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

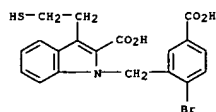
L11 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 560131-42-2 HCAPLUS
CN 1H-Indole-2,7-dicarboxylic acid, 3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)



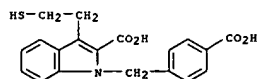
RN 560131-44-4 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 1-[(3-carboxyphenyl)methyl]-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)



RN 560131-46-6 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 1-[(2-bromo-5-carboxyphenyl)methyl]-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)



RN 560131-47-7 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 1-[(4-carboxyphenyl)methyl]-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)



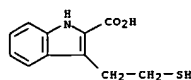
RN 560131-48-8 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 3-(2-mercaptoethyl)-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

L11 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

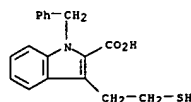
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003057670	A2	20030717	WO 2002-US37617	20021219
WO 2003057670	A3	20031106		
V: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BS, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, EC, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, NO, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GM, GQ, GW, ML, MR, NE, NG, SN, TD, TG				
AU 2002357003	A1	20030724	AU 2002-357003	20021219
US 2005080128	A1	20050414	US 2003-500319	20021219
PRIORITY APPLN. INFO.: US 2001-342764P P 20011228				
WO 2002-US37617 W 20021219				

OTHER SOURCE(S): MARPAT 139:101027
IT 560131-39-7P, 3-(2-Mercaptoethyl)-1H-indole-2-carboxylic acid
560131-42-2P, 3-(2-Mercaptoethyl)-1H-indole-2,7-dicarboxylic acid
560131-44-4P, 1-[(3-Carboxyphenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-46-6P, 1-[(2-bromo-5-carboxyphenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-47-7P, 1-[(4-Carboxyphenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-48-8P, 3-(2-Mercaptoethyl)-1-(phenylmethyl)-1H-indole-2-carboxylic acid 560131-49-9P, 1-[(2-Carboxyphenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-50-2P, 1-[(3-Carboxy-5-(1,1-dimethylethyl)phenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-51-3P, 1-[(4-Bromo-3-carboxyphenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-52-4P, 1-[(2-Carboxy-5-methoxyphenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-53-5P, 3-(2-Mercaptoethyl)-1-(2-phenylethyl)-1H-indole-2-carboxylic acid 560131-54-6P, 3-(2-Mercaptoethyl)-1-phenyl-1H-indole-2-carboxylic acid 560131-56-8P, 1-(3-Carboxyphenyl)-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-65-9P, 1-[3-Carboxy-5-(1,1-dimethylethyl)phenyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid R1: DGM (Diagnostic use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate and diagnosis agent; preparation of mercaptoethyl indolecarboxylic acids as NAALADase inhibitors for treating and diagnosing glutamate abnormalities and neurol. and other disorders)

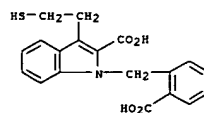
RN 560131-39-7 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)



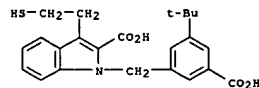
L11 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



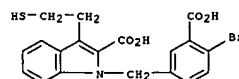
RN 560131-49-9 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 1-[(2-carboxyphenyl)methyl]-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)



RN 560131-50-2 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 1-[(3-carboxy-5-(1,1-dimethylethyl)phenyl)methyl]-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)

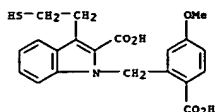


RN 560131-51-3 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 1-[(4-bromo-3-carboxyphenyl)methyl]-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)

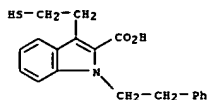


RN 560131-52-4 HCAPLUS
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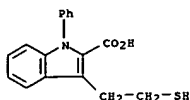
L11 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



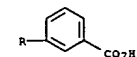
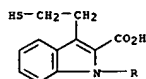
RN 560131-53-5 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 3-(2-mercaptoethyl)-1-(2-phenylethyl)- (9CI) (CA INDEX NAME)



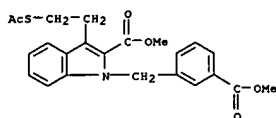
RN 560131-54-6 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 3-(2-mercaptoethyl)-1-phenyl- (9CI) (CA INDEX NAME)



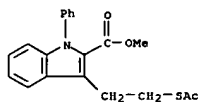
RN 560131-56-8 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 1-(3-carboxyphenyl)-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)



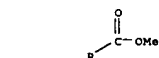
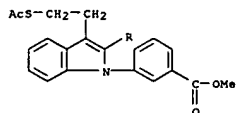
L11 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 560131-55-7 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 3-(2-(acetylthio)ethyl)-1-phenyl-, methyl ester (9CI) (CA INDEX NAME)

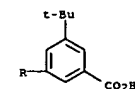
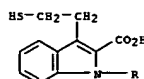


RN 560131-63-7 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 3-(2-(acetylthio)ethyl)-1-(3-(methoxycarbonyl)phenyl)-, methyl ester (9CI) (CA INDEX NAME)



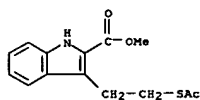
L11 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 560131-65-9 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 1-(3-carboxy-5-(1,1-dimethylethyl)phenyl)-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)



IT 560131-41-1F, Methyl 3-(2-(acetylthio)ethyl)-1H-indole-2-carboxylate 560131-45-5F, Methyl 3-(2-(acetylthio)ethyl)-1-[[3-(methoxycarbonyl)phenyl]methyl]-1H-indole-2-carboxylate 560131-55-7F, 3-(2-Acetylthioethyl)-1-phenyl-1H-indole-2-carboxylic acid methyl ester 560131-63-7F, 3-(2-Acetylsulfanylethyl)-1-[3-(methoxycarbonyl)phenyl]-1H-indole-2-carboxylic acid methyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of mercaptoethyl indolecarboxylic acids as NAALAdase inhibitors for treating and diagnosing glutamate abnormalities and neurol. and other disorders)

RN 560131-41-1 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 3-(2-(acetylthio)ethyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 560131-45-5 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 3-(2-(acetylthio)ethyl)-1-[[3-(methoxycarbonyl)phenyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

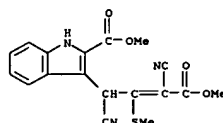
L11 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 12 May 1984
GI For diagram(s), see printed CA Issue.
AB 2,2-Bis(methylthio)-1-(1-methyl-2-methoxycarbonylindol-3-yl)acrylonitrile (I) reacted with amines, to give B-carboline derivs. 1,3-Dioxo-β-carboline derivs. were obtained by treatment of I with polyphosphoric acid. 1,3-Dioxo-β-carboline treated with CS₂ and NaH and alkylated with Me₂SO₄ gave 1,3-dioxo-1,3,4-trihydro-2,9-dimethyl -4-[bis(methylthio)methylene] -β- carboline. Reaction of 3-cyanomethylindole derivs. and ketene thioacetals afforded II (R = Me, Et; R₁ = CO₂Me, CN), 1-cyano-2-(methylthio)-3-nitro-4-hydroxycarbazole, and 1-oxo-1,2,9-trihydro-3-(methylthio)-4-cyano-β-carboline.

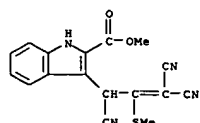
ACCESSION NUMBER: 1972:488363 HCAPLUS
DOCUMENT NUMBER: 77:88363
TITLE: Indole derivatives. XIII. Reaction of 1-(1-methyl-2-methoxycarbonylindol-3-yl)-2,2-bismethylthioacrylonitrile
AUTHOR(S): Kobayashi, Goro; Matsuda, Yoshiro; Matsuki, Reiko; Tominaga, Yoshinori
CORPORATE SOURCE: Pharm. Fac., Univ. Nagasaki, Nagasaki, Japan
SOURCE: Yakugaku Zasshi (1972), 92(6), 713-18
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

IT 37024-05-8F 37024-06-8F 37024-07-0F
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 37024-05-8 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 3-[1,3,3-tricyano-2-(methylthio)-4-oxo-2-butenyl]-, methyl ester (9CI) (CA INDEX NAME)



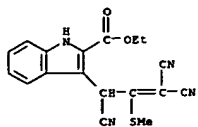
RN 37024-06-9 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 3-[1,3,3-tricyano-2-(methylthio)-2-propenyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 37024-07-0 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 3-[1,3,3-tricyano-2-(methylthio)-2-propenyl]-, ethyl ester (9CI) (CA INDEX NAME)

10500319

L11 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



10500319

=> d his

(FILE 'HOME' ENTERED AT 11:15:52 ON 08 JUN 2006)

FILE 'REGISTRY' ENTERED AT 11:16:04 ON 08 JUN 2006

L1 STRUCTURE UPLOADED
L2 2 S L1
L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 11:16:39 ON 08 JUN 2006

L4 1 S L3

FILE 'REGISTRY' ENTERED AT 11:17:06 ON 08 JUN 2006

L5 STRUCTURE UPLOADED
L6 3 S L5
L7 21 S L5 FULL
L8 STRUCTURE UPLOADED
L9 50 S L8
L10 3611 S L8 FULL

FILE 'HCAPLUS' ENTERED AT 11:21:45 ON 08 JUN 2006

L11 2 S L7

=> s l10

L12 880 L10

=> s l12 and (indole-2-carboxylic)

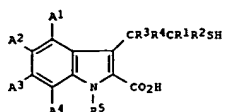
60043 INDOLE
8759472 2
238337 CARBOXYLIC
1295 INDOLE-2-CARBOXYLIC
(INDOLE(W) 2 (W) CARBOXYLIC)
L13 157 L12 AND (INDOLE-2-CARBOXYLIC)

=> s l13 and (mercapto?)

117655 MERCAPTO?
L14 10 L13 AND (MERCAPTO?)

=> d ed abs ibib hitstr 1-10

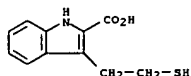
L14 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN
 ED Entered STN: 18 Jul 2003
 GI



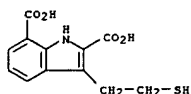
AB This invention relates to new indoles (shown as I; variables defined below; e.g. 3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid), pharmaceutical compns. and diagnostic kits comprising such compds., and methods of using such compds. for inhibiting NAALADase enzyme activity, detecting diseases where NAALADase levels are altered, affecting neuronal activity, effecting TGF- β activity, inhibiting angiogenesis, and treating glutamate abnormalities, neuropathy, pain, compulsive disorders, prostate diseases, cancers and glaucoma. IC50 values are tabulated for inhibition of NAALADase by 12 examples of I. Many pharmacol. and therapeutic test results are reported for the following 6 compds. that are not covered by I: 2-[[2,3,4,5,6-pentafluorobenzyl]hydroxyphosphinyl]methyl]pentanedioic acid, 2-(3-sulfanylpropyl)pentanedioic acid, 2-(phosphonomethyl)pentanedioic acid, 2-(2-sulfanylethyl)pentanedioic acid, 3-carboxy- α -(3-mercaptoethyl)benzenepropanoic acid and 3-carboxy-5-(1,1-dimethylethyl)- α -(3-mercaptoethyl)benzenepropanoic acid. For I: A1, A2, A3 and A4 = H, C1-C9 alkyl, C2-C9 alkenyl, C2-C9 alkynyl, aryl, heteroaryl, carbocycle, heterocycle, C1-C9 alkoxy, C2-C9 alkenyloxy, phenoxy, benzyloxy, hydroxy, halo, nitro, cyano, isocyano, -COOR6, -COR6, -NR6R7, -SR6, -SOR6, -SO2R6, -SO2(OR6), -C(O)NR6R7, -C(O)NR6 (CH2)nCOOH, -NR6C(O)R7 or -(CH2)nCOOH, or any adjacent two of A1, A2, A3 and A4 form with the benzene ring a fused ring that is (un)saturated, aromatic or nonarom., and carbocyclic or heterocyclic, said heterocyclic ring containing 1 or 2 O, N and/or S heteroatom(s); n is 1-3; R, R1, R2, R3, R4, R5, R6, R7 = H, carboxy, C1-C9 alkyl, C2-C9 alkenyl, C2-C9 alkynyl, aryl, heteroaryl, carbocycle or heterocycle; and said alkyl, alkenyl, alkynyl, aryl, heteroaryl, carbocycle, heterocycle, alkoxy, alkenyloxy, phenoxy, benzyloxy and fused ring (un)substituted with ≥ 1 substituent(s). Although the methods of preparation are not claimed, 13 example preps. are included.

ACCESSION NUMBER: 2003:551494 HCAPLUS
 DOCUMENT NUMBER: 139:101027
 TITLE: Preparation of mercaptoethyl indolecarboxylic acids as NAALADase inhibitors for treating and diagnosing glutamate abnormalities, neurological and other disorders
 INVENTOR(S): Tsukamoto, Takashi; Grella, Brian; Majer, Pavel
 PATENT ASSIGNEE(S): Guilford Pharmaceuticals Inc., USA
 SOURCE: PCT Int. Appl., 173 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1

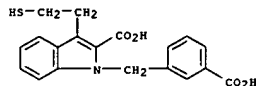
L14 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



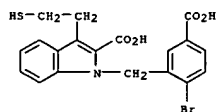
RN 560131-42-2 HCAPLUS
 CN 1H-Indole-2,7-dicarboxylic acid, 3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)



RN 560131-44-4 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[(3-carboxyphenyl)methyl]-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)



RN 560131-46-6 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[(2-bromo-5-carboxyphenyl)methyl]-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)



RN 560131-47-7 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[(4-carboxyphenyl)methyl]-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)

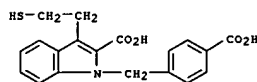
L14 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PATENT INFORMATION:

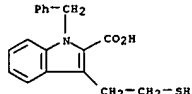
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003057670	A2	20030717	WO 2002-0537617	20021219
WO 2003057670	A3	20031106		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SS, SZ, TG, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, NO, NZ, PL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, HT, IL, IN, KE, NE, NG, SD, TD, TG				
AU 2002357003	A1	20030724	AU 2002-357003	20021219
US 2005080128	A1	20050414	US 2003-500139	20021219
PRIORITY APPLN. INFO.:				US 2001-34764P
				WO 2002-0537617
				P 20011228
				W 20021219

OTHER SOURCE(S): MARPAT 139:101027
 IT 560131-39-7P, 3-(2-Mercaptoethyl)-1H-indole-2-carboxylic acid 560131-42-2P, 3-(2-Mercaptoethyl)-1H-indole-2,7-dicarboxylic acid 560131-44-4P, 1-[(3-Carboxyphenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-46-6P, 1-[(2-Bromo-5-carboxyphenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-47-7P, 1-[(4-Carboxyphenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-48-8P, 3-(2-Mercaptoethyl)-1-1-(phenylethyl)-1H-indole-2-carboxylic acid 560131-49-9P, 1-[(2-Carboxyphenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-50-2P, 1-[(3-Carboxy-5-(1,1-dimethylethyl)phenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-51-3P, 1-[(4-Bromo-3-carboxyphenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-52-4P, 1-[(2-Carboxy-5-methoxyphenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-53-5P, 3-(2-Mercaptoethyl)-1-(2-phenylethyl)-1H-indole-2-carboxylic acid 560131-54-6P, 3-(2-Mercaptoethyl)-1-phenyl-1H-indole-2-carboxylic acid 560131-56-8P, 1-(3-Carboxyphenyl)-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid 560131-65-9P, 1-[(3-Carboxy-5-(1,1-dimethylethyl)phenyl)methyl]-3-(2-mercaptoethyl)-1H-indole-2-carboxylic acid
 RI: DGN (Diagnostic use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (drug candidate and diagnosis agent; preparation of mercaptoethyl indolecarboxylic acids as NAALADase inhibitors for treating and diagnosing glutamate abnormalities and neurol. and other disorders)
 RN 560131-39-7 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)

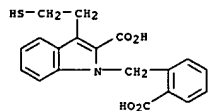
L14 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



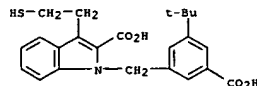
RN 560131-48-8 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 3-(2-mercaptoethyl)-1-(phenylethyl)- (9CI) (CA INDEX NAME)



RN 560131-49-9 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[(2-carboxyphenyl)methyl]-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)

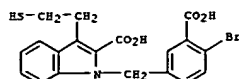


RN 560131-50-2 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[(3-carboxy-5-(1,1-dimethylethyl)phenyl)methyl]-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)

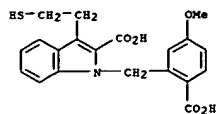


RN 560131-51-3 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[(4-bromo-3-carboxyphenyl)methyl]-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)

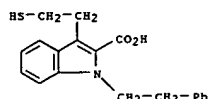
L14 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



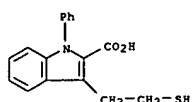
RN 560131-52-4 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 1-((2-carboxy-5-methoxyphenyl)methyl)-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)



RN 560131-53-5 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 3-(2-mercaptoethyl)-1-(2-phenylethyl)- (9CI) (CA INDEX NAME)



RN 560131-54-6 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 3-(2-mercaptoethyl)-1-phenyl- (9CI) (CA INDEX NAME)



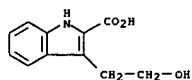
RN 560131-56-8 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 1-(3-carboxyphenyl)-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)

L14 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

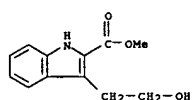
carboxylic acid 560131-40-0P, Methyl 3-(2-Hydroxyethyl)-1H-indole-2-carboxylate 560131-41-1P, Methyl 3-(2-(acetylthio)ethyl)-1H-indole-2-carboxylate 560131-45-5P, Methyl 3-(2-(acetylthio)ethyl)-1-[[3-(methoxycarbonyl)phenyl]methyl]-1H-indole-2-carboxylate 560131-55-7P, 3-(2-Acetylthioethyl)-1-phenyl-1H-indole-2-carboxylic acid methyl ester 560131-57-9P, 3-[(ethoxycarbonyl)methyl]-1-[3-(methoxycarbonyl)phenyl]-1H-indole-2-carboxylic acid ethyl ester 560131-58-0P, 3-Carboxymethyl-1-(3-carboxyphenyl)-1H-indole-2-carboxylic acid 560131-59-1P, 1-(3-Carboxyphenyl)-3-[(ethoxycarbonyl)methyl]-1H-indole-2-carboxylic acid 560131-60-4P, 1-(3-Carboxyphenyl)-3-(2-hydroxyethyl)-1H-indole-2-carboxylic acid 560131-61-5P, 3-(2-Hydroxyethyl)-1-[3-(methoxycarbonyl)phenyl]-1H-indole-2-carboxylic acid methyl ester 560131-62-6P, 1-[3-(Methoxycarbonyl)phenyl]-3-[2-(4-tolylsulfonyloxy)ethyl]-1H-indole-2-carboxylic acid methyl ester 560131-63-7P, 3-(2-Acetylsulfanylethyl)-1-[3-(methoxycarbonyl)phenyl]-1H-indole-2-carboxylic acid methyl ester

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of mercaptoethyl indolecarboxylic acids as NAALadase inhibitors for treating and diagnosing glutamate abnormalities and neurol. and other disorders)

RN 77903-96-9 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 3-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)

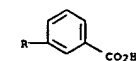
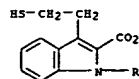


RN 560131-40-0 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 3-(2-hydroxyethyl)-, methyl ester (9CI) (CA INDEX NAME)

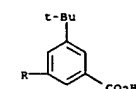
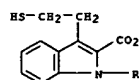


RN 560131-41-1 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 3-(2-(acetylthio)ethyl)-, methyl ester (9CI) (CA INDEX NAME)

L14 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

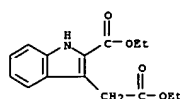


RN 560131-65-9 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 1-(3-carboxy-5-(1,1-dimethylethyl)phenyl)-3-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)



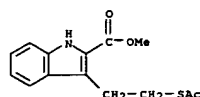
IT 63158-60-1, [2-(Ethoxycarbonyl)indol-3-yl]acetic acid ethyl ester
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of mercaptoethyl indolecarboxylic acids as NAALadase inhibitors for treating and diagnosing glutamate abnormalities and neurol. and other disorders)

RN 63158-60-1 HCAPLUS
CN 1H-Indole-3-acetic acid, 2-(ethoxycarbonyl)-, ethyl ester (9CI) (CA INDEX NAME)

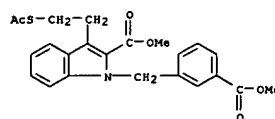


IT 77903-96-9P, 3-(2-Hydroxyethyl)-1H-indole-2-

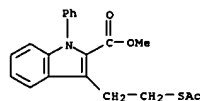
L14 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



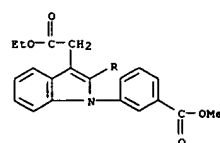
RN 560131-45-5 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 3-(2-(acetylthio)ethyl)-1-phenyl-, methyl ester (9CI) (CA INDEX NAME)



RN 560131-55-7 HCAPLUS
CN 1H-Indole-2-carboxylic acid, 3-(2-(acetylthio)ethyl)-1-phenyl-, methyl ester (9CI) (CA INDEX NAME)

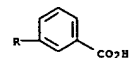
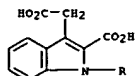


RN 560131-57-9 HCAPLUS
CN 1H-Indole-3-acetic acid, 2-(ethoxycarbonyl)-1-[3-(methoxycarbonyl)phenyl]-, ethyl ester (9CI) (CA INDEX NAME)

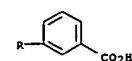
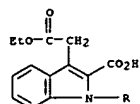


L14 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 560131-58-0 HCAPLUS
 CN 1H-Indole-3-acetic acid, 2-carboxy-1-(3-carboxyphenyl)- (9CI) (CA INDEX NAME)

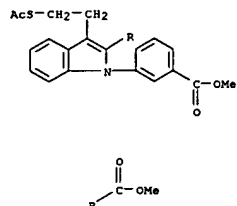


RN 560131-59-1 HCAPLUS
 CN 1H-Indole-3-acetic acid, 2-carboxy-1-(3-carboxyphenyl)-, alpha-ethyl ester (9CI) (CA INDEX NAME)

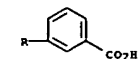
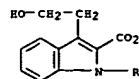


RN 560131-60-4 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-(3-carboxyphenyl)-3-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)

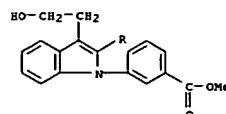
L14 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 CN 1H-Indole-2-carboxylic acid, 3-[2-(acetylthio)ethyl]-1-[3-(methoxycarbonyl)phenyl]-, methyl ester (9CI) (CA INDEX NAME)



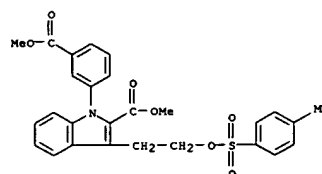
L14 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 560131-61-5 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 3-(2-hydroxyethyl)-1-[3-(methoxycarbonyl)phenyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 560131-62-6 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[3-(methoxycarbonyl)phenyl]-3-[2-[[4-methylphenyl)sulfonyl]oxy]ethyl]-, methyl ester (9CI) (CA INDEX NAME)



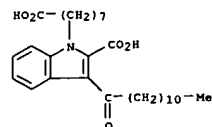
RN 560131-63-7 HCAPLUS

L14 ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN

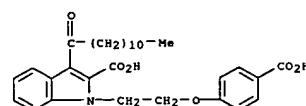
ED Entered STN: 14 Sep 2001

AB Derivs. of 1-[2-(4-carboxyphenoxy)ethyl]-3-(1-oxododecyl)-1H-indole-2-carboxylic acid with modified substituents at the indole 1-position were synthesized and evaluated for their ability to inhibit the arachidonic acid release in human platelets mediated by the cytosolic phospholipase A2. One of the most active compds. was 1-[2-(4-carboxy-2-fluorophenoxy)ethyl]-3-(1-oxododecyl)-1H-indole-2-carboxylic acid with an IC50 of 0.44 μM.

ACCESSION NUMBER: 2001:674620 HCAPLUS
 DOCUMENT NUMBER: 136:85739
 TITLE: Novel 3-dodecanoylindole-2-carboxylic acid inhibitors of cytosolic phospholipase A2
 AUTHOR(S): Lehr, M.; Klimt, M.; Elfringhoff, A. S.
 CORPORATE SOURCE: Institute of Pharmaceutical Chemistry, University of Munster, Munster, D-48149, Germany
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2001), 11(19), 2569-2572
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 136:85739
 IT 192182-27-7D, docexanoylindole-2-carboxylic acid derivative
 192182-43-7D, docexanoylindole-2-carboxylic acid derivative
 192182-47-1D, docexanoylindole-2-carboxylic acid derivative
 RL: BSU (Biological study, unclassified); BIOL (Biological study) (preparation of 3-(1-oxododecyl)-1H-indole-2-carboxylates as inhibitors of cytosolic phospholipase A2)
 RN 192182-27-7 HCAPLUS
 CN 1H-Indole-1-octanoic acid, 2-carboxy-3-(1-oxododecyl)- (9CI) (CA INDEX NAME)

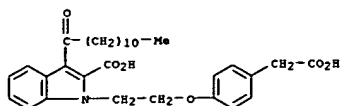


RN 192182-43-7 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[2-(4-carboxyphenoxy)ethyl]-3-(1-oxododecyl)- (9CI) (CA INDEX NAME)

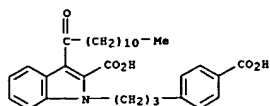


RN 192182-47-1 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[2-[4-(carboxymethyl)phenoxy]ethyl]-3-(1-

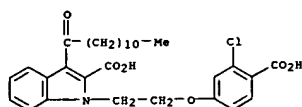
L14 ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



IT 205106-44-1P 205106-45-2P 205106-46-3P
 205106-47-4P 205106-48-5P 386213-03-2P
 386213-09-8P 386213-10-1P 386213-11-2P
 386213-12-3P 386213-13-4P 386213-14-5P
 386213-15-6P 386213-16-7P 386213-17-8P
 386213-18-9P 386213-19-0P 386213-20-3P
 RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);
 BIOL (Biological study); PREP (Preparation)
 (preparation of 3-(1-oxododecyl)-1H-indole-2-carboxylates as inhibitors of
 cytosolic phospholipase A2)
 RN 205106-44-1 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[3-(4-carboxyphenyl)propyl]-3-(1-oxododecyl)- (9CI) (CA INDEX NAME)

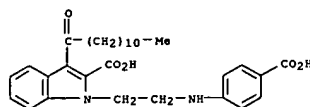


RN 205106-45-2 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[2-(4-carboxy-3-chlorophenoxy)ethyl]-3-(1-oxododecyl)- (9CI) (CA INDEX NAME)

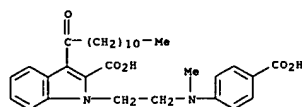


RN 205106-46-3 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[2-(4-carboxy-2-chlorophenoxy)ethyl]-3-(1-oxododecyl)- (9CI) (CA INDEX NAME)

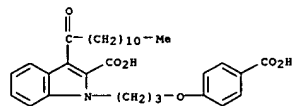
L14 ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



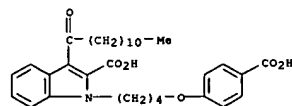
RN 386213-10-1 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[2-((4-carboxyphenyl)methylamino)ethyl]-3-(1-oxododecyl)- (9CI) (CA INDEX NAME)



RN 386213-11-2 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[3-(4-carboxyphenoxy)propyl]-3-(1-oxododecyl)- (9CI) (CA INDEX NAME)

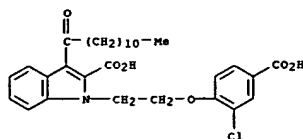


RN 386213-12-3 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[4-(4-carboxyphenoxy)butyl]-3-(1-oxododecyl)- (9CI) (CA INDEX NAME)

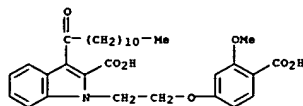


RN 386213-13-4 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[2-(4-carboxy-2-methoxyphenoxy)ethyl]-3-(1-oxododecyl)- (9CI) (CA INDEX NAME)

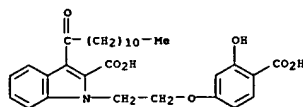
L14 ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



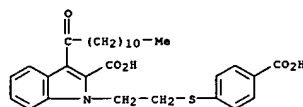
RN 205106-47-4 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[2-(4-carboxy-3-methoxyphenoxy)ethyl]-3-(1-oxododecyl)- (9CI) (CA INDEX NAME)



RN 205106-48-5 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[2-(4-carboxy-3-hydroxyphenoxy)ethyl]-3-(1-oxododecyl)- (9CI) (CA INDEX NAME)

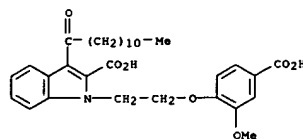


RN 386213-03-2 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[2-((4-carboxyphenyl)thio)ethyl]-3-(1-oxododecyl)- (9CI) (CA INDEX NAME)

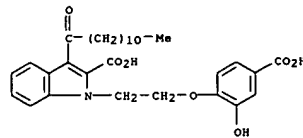


RN 386213-09-8 HCAPLUS

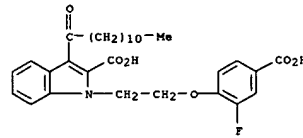
L14 ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 386213-14-5 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[2-(4-carboxy-2-hydroxyphenoxy)ethyl]-3-(1-oxododecyl)- (9CI) (CA INDEX NAME)

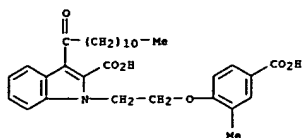


RN 386213-15-6 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[2-(4-carboxy-2-fluorophenoxy)ethyl]-3-(1-oxododecyl)- (9CI) (CA INDEX NAME)

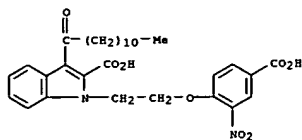


RN 386213-16-7 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[2-(4-carboxy-2-methylphenoxy)ethyl]-3-(1-oxododecyl)- (9CI) (CA INDEX NAME)

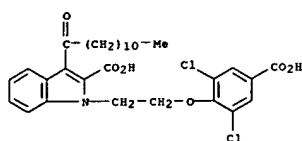
L14 ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 386213-17-8 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[2-(4-carboxy-2-nitrophenoxy)ethyl]-3-(1-oxododecyl)- (9CI) (CA INDEX NAME)

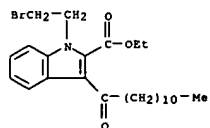


RN 386213-18-9 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[2-(4-carboxy-2,6-dichlorophenoxy)ethyl]-3-(1-oxododecyl)- (9CI) (CA INDEX NAME)



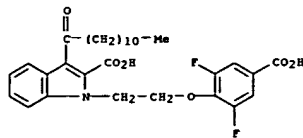
RN 386213-19-0 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[2-(4-carboxy-2,6-difluorophenoxy)ethyl]-3-(1-oxododecyl)- (9CI) (CA INDEX NAME)

L14 ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

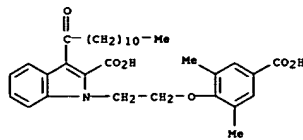


REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

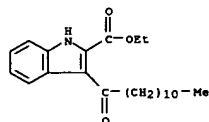
L14 ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 386213-20-3 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[2-(4-carboxy-2,6-dimethylphenoxy)ethyl]-3-(1-oxododecyl)- (9CI) (CA INDEX NAME)

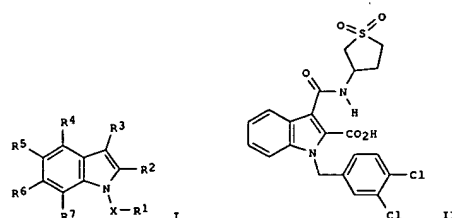


IT 203111-21-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of 3-(1-oxododecyl)-1H-indole-2-carboxylates as inhibitors of cytosolic phospholipase A2)
 RN 203111-21-1 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 3-(1-oxododecyl)-, ethyl ester (9CI) (CA INDEX NAME)



IT 386213-02-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of 3-(1-oxododecyl)-1H-indole-2-carboxylates as inhibitors of cytosolic phospholipase A2)
 RN 386213-02-1 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-(2-bromoethyl)-3-(1-oxododecyl)-, ethyl ester (9CI) (CA INDEX NAME)

L14 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN
 ED Entered STN: 11 Aug 2000
 GI



AB The title compds. [I; X = CH₂, SO₂; R₁ = (un)substituted aryl, heteroaryl; R₂ = CO₂H, CN, COCH₂OH, etc.; R₃ = OR₁₅ (wherein R₁₅ = substituted alkyl or cycloalkyl, (un)substituted heteroaryl), S(O)qR₁₅ (q = 0-2), (CH₂)sCO₂H (s = 0-4), etc.; R₄-R₇ = H, (un)substituted hydrocarbyl, heterocyclyl, etc.] and their pharmaceutically acceptable salts, amides or esters, useful in the preparation of a medicament for the inhibition of monocyte chemoattractant protein-1 and/or RANTES induced chemotaxis, were prepared and formulated. Thus, hydrolysis of the corresponding ester afforded 93% II which showed IC₅₀ of 6.86 μM against hMCP-1 receptor binding.

ACCESSION NUMBER: 2000:553556 HCAPLUS
 DOCUMENT NUMBER: 133:150463
 TITLE: Preparation of 3-substituted indole-2-carboxylic acids for the inhibition of monocyte chemoattractant protein-1 and/or RANTES induced chemotaxis
 INVENTOR(S): Faull, Alan Wellington; Kettle, Jason
 PATENT ASSIGNEE(S): AstraZeneca UK Limited, UK
 SOURCE: PCT Int. Appl., 72 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000046199	A2	20000810	WO 2000-GB284	20000131
WO 2000046199	A3	20001130		
W: AE, AL, AM, AT, AU, A2, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, K2, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, T2, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2355734	AA	20000810	CA 2000-2355734	20000131
BR 2000008015	A	20011106	BR 2000-8015	20000131

L14 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 EP 1173421 A2 20020123 EP 2000-901747 20000131
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO
 JP 2002536362 T2 20021029 JP 2000-597270 20000131
 ZA 2001005017 A 20020919 ZA 2001-5017 20010619
 NO 2001003768 A 20011001 NO 2001-3768 20010801
 US 6933397 B1 20041221 US 2001-89516 20011002
 PRIORITY APPLN. INFO.: GB 1999-2455 A 19990205
 WO 2000-GB284 W 20000131

OTHER SOURCE(S): MARPAT 133:150463

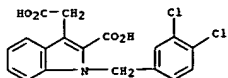
IT 287725-35-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of 3-substituted indole-2-carboxylic acids for the inhibition of monocyte chemoattractant protein-1 and/or RANTES induced chemotaxis)

RN 287725-35-3 HCAPLUS

CN 1H-Indole-3-acetic acid, 2-carboxy-1-[(3,4-dichlorophenyl)methyl]- (9CI) (CA INDEX NAME)



IT 287725-55-7P 287725-56-8P 287725-57-9P

287725-59-1P 287725-60-4P 287725-61-5P

287725-62-6P 287725-63-7P 287725-64-8P

287725-65-9P 287725-66-0P 287725-67-1P

287725-68-2P 287725-69-3P 287725-70-6P

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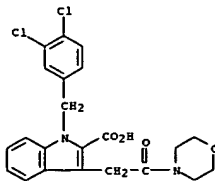
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 3-substituted indole-2-carboxylic acids for the inhibition of monocyte chemoattractant protein-1 and/or RANTES induced chemotaxis)

RN 287725-55-7 HCAPLUS

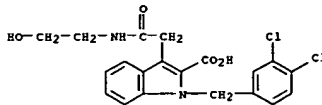
CN 1H-Indole-2-carboxylic acid, 1-[(3,4-dichlorophenyl)methyl]-3-[2-(4-morpholinyl)-2-oxoethyl]- (9CI) (CA INDEX NAME)

L14 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 287725-56-8 HCAPLUS

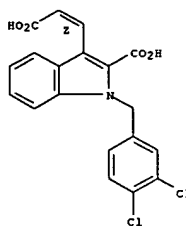
CN 1H-Indole-2-carboxylic acid, 1-[(3,4-dichlorophenyl)methyl]-3-[2-[(2-hydroxyethyl)amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)



RN 287725-57-9 HCAPLUS

CN 1H-Indole-2-carboxylic acid, 3-[(1E)-2-carboxyethenyl]-1-[(3,4-dichlorophenyl)methyl]- (9CI) (CA INDEX NAME)

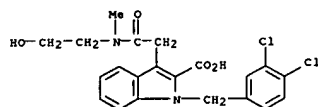
Double bond geometry as shown.



RN 287725-59-1 HCAPLUS

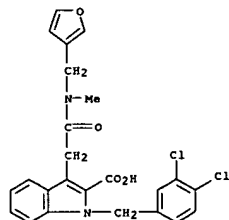
CN 1H-Indole-2-carboxylic acid, 1-[(3,4-dichlorophenyl)methyl]-3-[2-[(2-hydroxyethyl)methylamino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

L14 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



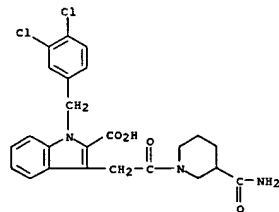
RN 287725-60-4 HCAPLUS

CN 1H-Indole-2-carboxylic acid, 1-[(3,4-dichlorophenyl)methyl]-3-[2-[(3-furanylmethyl)methylamino]-2-oxoethyl]- (9CI) (CA INDEX NAME)



RN 287725-61-5 HCAPLUS

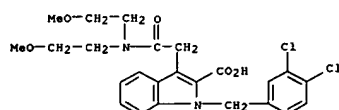
CN 1H-Indole-2-carboxylic acid, 3-[2-[(3-(aminocarbonyl)-1-piperidinyl)-2-oxoethyl]-1-[(3,4-dichlorophenyl)methyl]- (9CI) (CA INDEX NAME)



RN 287725-62-6 HCAPLUS

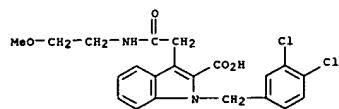
CN 1H-Indole-2-carboxylic acid, 3-[2-[(bis(2-methoxyethyl)amino)-2-oxoethyl]-1-[(3,4-dichlorophenyl)methyl]- (9CI) (CA INDEX NAME)

L14 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



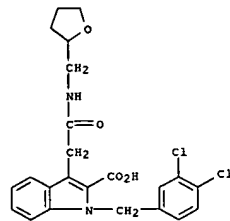
RN 287725-63-7 HCAPLUS

CN 1H-Indole-2-carboxylic acid, 1-[(3,4-dichlorophenyl)methyl]-3-[2-[(2-methoxyethyl)amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)



RN 287725-64-8 HCAPLUS

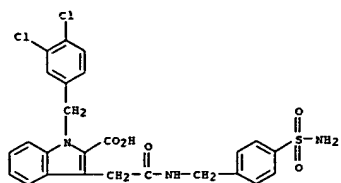
CN 1H-Indole-2-carboxylic acid, 1-[(3,4-dichlorophenyl)methyl]-3-[2-oxo-2-[(tetrahydro-2-furanyl)methyl]amino]ethyl]- (9CI) (CA INDEX NAME)



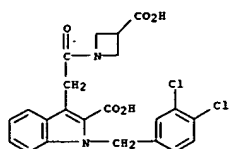
RN 287725-65-9 HCAPLUS

CN 1H-Indole-2-carboxylic acid, 3-[2-[(4-(aminosulfonyl)phenyl)methyl]amino]-2-oxoethyl]-1-[(3,4-dichlorophenyl)methyl]- (9CI) (CA INDEX NAME)

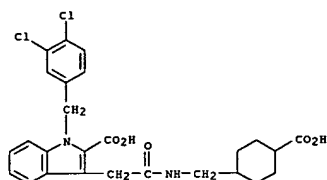
L14 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 287725-66-0 HCAPLUS
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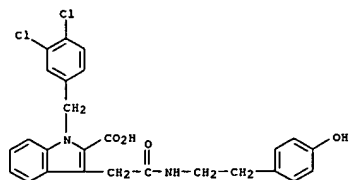


RN 287725-67-1 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 3-[2-(((4-carboxycyclohexyl)methyl)amino)-2-oxoethyl]-1-[(3,4-dichlorophenyl)methyl]- (9CI) (CA INDEX NAME)

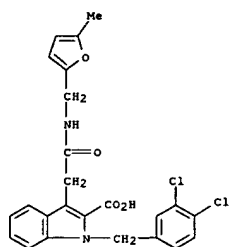


RN 287725-68-2 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 3-[2-([2-(4-(aminosulfonyl)phenyl)ethyl]amino)-2-oxoethyl]-1-[(3,4-dichlorophenyl)methyl]- (9CI) (CA INDEX NAME)

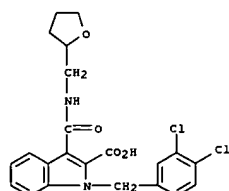
L14 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 287725-72-8 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[(3,4-dichlorophenyl)methyl]-3-[2-(((5-methyl-2-furanyl)methyl)amino)-2-oxoethyl]- (9CI) (CA INDEX NAME)

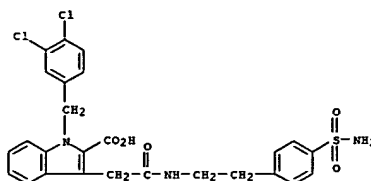


RN 287725-75-1 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[(3,4-dichlorophenyl)methyl]-3-[[[2-(tetrahydro-2-furanyl)methyl]amino]carbonyl]- (9CI) (CA INDEX NAME)

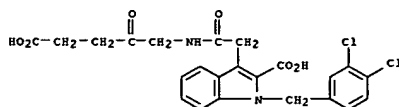


RN 287725-88-6 HCAPLUS

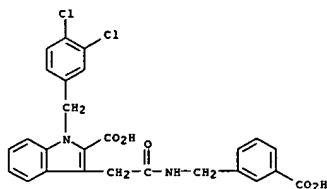
L14 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 287725-69-3 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 3-[2-((4-carboxy-2-oxobutyl)amino)-2-oxoethyl]-1-[(3,4-dichlorophenyl)methyl]- (9CI) (CA INDEX NAME)

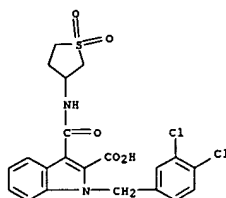


RN 287725-70-6 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 3-[2-(((3-carboxyphenyl)methyl)amino)-2-oxoethyl]-1-[(3,4-dichlorophenyl)methyl]- (9CI) (CA INDEX NAME)

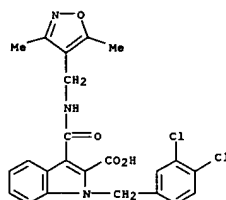


RN 287725-71-7 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[(3,4-dichlorophenyl)methyl]-3-[2-([2-(4-hydroxyphenyl)ethyl]amino)-2-oxoethyl]- (9CI) (CA INDEX NAME)

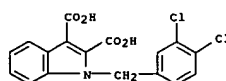
L14 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 CN 1H-Indole-2-carboxylic acid, 1-[(3,4-dichlorophenyl)methyl]-3-[[[2-(tetrahydro-1,1-dioxido-3-thienyl)amino]carbonyl]- (9CI) (CA INDEX NAME)



RN 287725-92-2 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[(3,4-dichlorophenyl)methyl]-3-[[[2-(3,5-dimethyl-4-isoxazolyl)methyl]amino]carbonyl]- (9CI) (CA INDEX NAME)

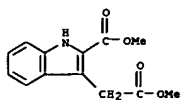


RN 287725-93-3 HCAPLUS
 CN 1H-Indole-2,3-dicarboxylic acid, 1-[(3,4-dichlorophenyl)methyl]- (9CI) (CA INDEX NAME)

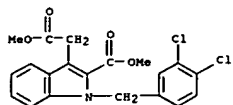


IT 156362-00-4P 287726-00-5P 287726-02-7P
 287726-46-8P 287726-47-0P 287726-49-2P
 287726-50-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of 3-substituted indole-2-carboxylic acids for the inhibition of monocyte chemoattractant

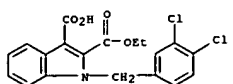
L14 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 protein-1 and/or RANTES induced Chemotaxis)
 RN 156362-00-4 HCAPLUS
 CN 1H-Indole-3-acetic acid, 2-(methoxycarbonyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 287726-00-5 HCAPLUS
 CN 1H-Indole-3-acetic acid, 1-[(3,4-dichlorophenyl)methyl]-2-(methoxycarbonyl)-, methyl ester (9CI) (CA INDEX NAME)

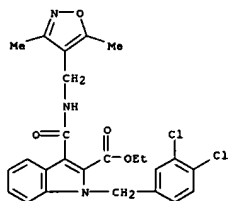


RN 287726-02-7 HCAPLUS
 CN 1H-Indole-2,3-dicarboxylic acid, 1-[(3,4-dichlorophenyl)methyl]-, 2-ethyl ester (9CI) (CA INDEX NAME)



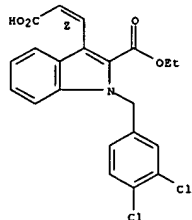
RN 287726-46-9 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[(3,4-dichlorophenyl)methyl]-3-[[[(tetrahydro-2-furanyl)methyl]amino]carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)

L14 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

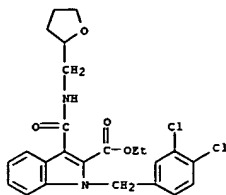


RN 287726-50-5 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 3-[(1Z)-2-carboxyethenyl]-1-[(3,4-dichlorophenyl)methyl]-, 2-ethyl ester (9CI) (CA INDEX NAME)

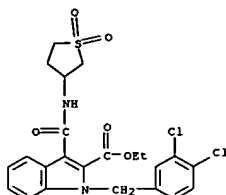
Double bond geometry as shown.



L14 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 287726-47-0 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[(3,4-dichlorophenyl)methyl]-3-[[[(tetrahydro-1,1-dioxido-3-thienyl)amino]carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 287726-49-2 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 1-[(3,4-dichlorophenyl)methyl]-3-[[[(3,5-dimethyl-4-isoxazolyl)methyl]amino]carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)

L14 ANSWER 4 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 26 May 2000

AB New therapies can be devised based upon a demonstration of the role of glutamate in the pathogenesis of cancer. Inhibitors of the interaction of glutamate with the AMPA, kainate, or NMDA receptor complexes are likely to be useful in treating cancer and can be formulated as pharmaceutical compns. They can be identified by appropriate screens.

ACCESSION NUMBER: 2000:351162 HCAPLUS

DOCUMENT NUMBER: 133:790

TITLE: New use of glutamate antagonists for the treatment of cancer

INVENTOR(S): Ikonomidou, Hrisanthi

PATENT ASSIGNEE(S): Germany

SOURCE: Eur. Pat. Appl., 21 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1002535	A1	20000524	EP 1998-250380	19981028
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
AU 9964750	A1	20000515	AU 1999-64750	19991022
EP 1124553	A1	20010822	EP 1999-952622	19991022
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002528415	T2	20020903	JP 2000-578005	19991022
EP 1586321	A1	20051019	EP 2005-12871	19991022
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
EP 1649857	A2	20060426	EP 2005-12872	19991022
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
US 6797692	B1	20040928	US 2001-830354	20010425
US 2005054619	A1	20050310	US 2004-912159	20040806
US 2005054650	A1	20050310	US 2004-912175	20040806
PRIORITY APPLN. INFO.:			EP 1998-250380	A 19981028
			EP 1999-952622	A3 19991022
			WO 1999-EP8004	W 19991022
			US 2001-830354	A3 20010425

IT 153436-38-5, GV150526 270902-31-3D, derivs.

270921-51-2D, derivs.

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(glutamate antagonists for cancer treatment)

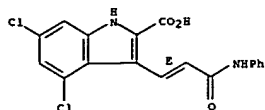
RN 153436-38-5 HCAPLUS

CN 1H-Indole-2-carboxylic acid, 4,6-dichloro-3-[(1E)-3-oxo-3-(phenylamino)-1-propenyl]-, monosodium salt (9CI) (CA INDEX NAME)

Double bond geometry as shown.

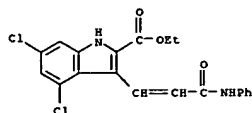
10500319

L14 ANSWER 4 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



● Na

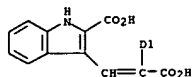
RN 270902-31-3 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 4,6-dichloro-3-[3-oxo-3-(phenylamino)-1-propenyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 270921-51-2 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 3-[2-(aminophenyl)-2-carboxyethenyl]- (9CI) (CA INDEX NAME)

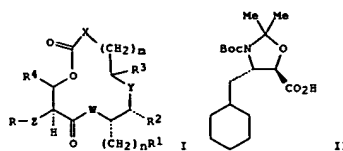


D1-NH2

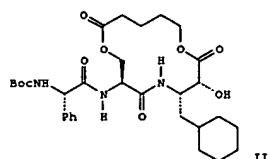


REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 5 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN
 ED Entered STN: 04 Sep 1993
 GI



II



III

AB Macrocyclic peptides I [e.g., R2 = Boc-Phe (Boc = Me3CO2C), (S)-1-[[4-(methoxymethoxy)piperidino]carbonyl]-2-phenylethoxy; W = O, NH, alkylimino; X = bond, CH2O, CH2S; Y = OCO, CH2CO, CH2CH(OH); R1 = alkyl, aryl, cycloalkyl, heterocyclyl; R2 = NH2, OH, OPO3H2, etc.; R3 = H, alkyl, substituted alkyl; R4 = alkyl, aryl, 4-imidazolyl, 4-thiazolyl, 5-thiazolyl; m = 1-4, n = 0-2] were prepared as renin inhibitors and are thus useful in treating, preventing, or managing renin-associated hypertension, hyperaldosterism, congestive heart failure, and glaucoma. Thus, oxalidinecarboxylic acid II was esterified with HO(CH2)mCO2CH2Ph and the ester coupled with PhCH2O2C-Ser-OCMe3. The product was deprotected with CF3CO2H/CH2Cl2 and underwent macrocyclization (by N-methylmorpholine, hydroxybenzotriazole, and substituted carbodiimide EDC) and coupling with Boc-Phe-OH to afford macrocycle III.

ACCESSION NUMBER: 1993:496178 HCAPLUS
 DOCUMENT NUMBER: 119:96178
 TITLE: Cyclic renin inhibitors
 INVENTOR(S): Greenlas, William J.; Patchett, Arthur A.; Weber, Ann E.; Tate, James R.
 PATENT ASSIGNEE(S): Merck and Co., Inc., USA
 SOURCE: Eur. Pat. Appl., 123 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

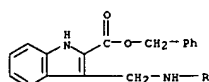
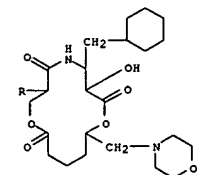
PATENT NO. KIND DATE APPLICATION NO. DATE

L14 ANSWER 5 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

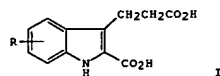
EP 518675 A2 19921216 EP 1992-305383 19920611
 EP 518675 A3 19930811
 R: CH, DE, FR, GB, IT, LI, NL
 CA 2070978 AA 19921212 CA 1992-2070978 19920610
 JP 06056807 A2 19940301 JP 1992-152087 19920611
 PRIORITY APPL. INFO.: US 1991-714112 A 19910611
 OTHER SOURCE(S): CASREACT 119:96178; MARPAT 119:96178

IT 137226-64-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation, hydrogenolysis of, and cyclodehydration of)

RN 137226-64-3 HCAPLUS
 CN 1H-Indole-2-carboxylic acid, 3-[[[6-(cyclohexylmethyl)-7-hydroxy-10-(4-morpholinylmethyl)-4,8,14-trioxo-1,9-dioxo-5-azacyclotetradec-3-yl]amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



L14 ANSWER 6 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN
 ED Entered STN: 27 Jun 1992
 GI

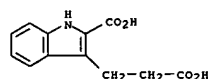


I

AB 3-(2-Carboxyindol-3-yl)propionic acids, e.g., I (R = H, Cl, F, OMe, NO2, CF3, OPh, NH2, etc.) were prepared from (un)substituted anilines or naphthylamines by Japp-Klingemann reaction and tested as antagonists for the strychnine-insensitive glycine binding site of the NMDA receptor. Chlorine, and other small electron-withdrawing substituents in the 4- and 6-positions of the indole ring, greatly enhanced binding and selectivity for the glycine site over the glutamate site of the NMDA receptor; one of the most potent compds. is 3-(4,6-dichloro-2-carboxyindol-3-yl)propionic acid (IC50 = 170 nM; >2100-fold selective for glycine). The importance of a heteroatom NH and the enhancing effect of the propionic acid side chain were demonstrated and are consistent with previous results which suggest the presence of a pocket on the receptor which can accept an acidic side chain. Substitution of a sulfur at C-3 led to the most potent compound, 3-[(carboxymethyl)thio]-2-carboxy-4,6-dichloroindole (IC50 = 100 nM).

ACCESSION NUMBER: 1992:255434 HCAPLUS
 DOCUMENT NUMBER: 116:255434
 TITLE: 3-(2-Carboxyindol-3-yl)propionic acid-based antagonists of the NMDA (N-methyl-D-aspartic acid) receptor associated glycine binding site
 AUTHOR(S): Salituro, Francesco G.; Harrison, Boyd L.; Baron, Bruce M.; Nyce, Philip L.; Stewart, Kenneth T.; Kehne, John H.; White, H. Steven; McDonald, Ian A.
 CORPORATE SOURCE: Marion Merrell Dow Res. Inst., Cincinnati, OH, 45215, USA
 SOURCE: Journal of Medicinal Chemistry (1992), 35(10), 1791-9
 CODEN: JMCHMR; ISSN: 0022-2623
 DOCUMENT TYPE: Journal
 LANGUAGE: English

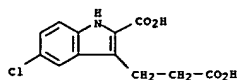
IT 31529-28-9P 54904-18-6P 130798-49-1P
 130798-50-4P 130798-51-5P 130942-03-9P
 132004-30-9P 132004-32-1P 132004-33-2P
 132004-34-3P 132004-35-4P 132004-36-5P
 139896-76-7P 139896-77-8P 139896-78-9P
 139896-79-0P 139896-80-3P 139896-81-4P
 139896-82-5P 139896-83-6P 139896-84-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and NMDA receptor antagonist activity of)
 RN 31529-28-9 HCAPLUS
 CN 1H-Indole-3-propanoic acid, 2-carboxy- (9CI) (CA INDEX NAME)



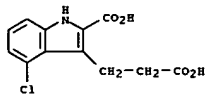
RN 54904-18-6 HCAPLUS

10500319

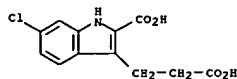
L14 ANSWER 6 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 1H-Indole-3-propanoic acid, 2-carboxy-5-chloro- (9CI) (CA INDEX NAME)



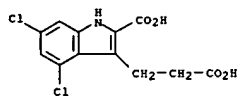
RN 130798-49-1 HCAPLUS
CN 1H-Indole-3-propanoic acid, 2-carboxy-4-chloro- (9CI) (CA INDEX NAME)



RN 130798-50-4 HCAPLUS
CN 1H-Indole-3-propanoic acid, 2-carboxy-6-chloro- (9CI) (CA INDEX NAME)

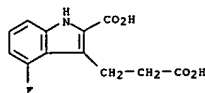


RN 130798-51-5 HCAPLUS
CN 1H-Indole-3-propanoic acid, 2-carboxy-4,6-dichloro- (9CI) (CA INDEX NAME)

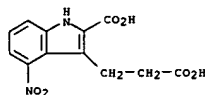


RN 130942-03-9 HCAPLUS
CN 1H-Indole-3-propanoic acid, 2-carboxy-7-chloro- (9CI) (CA INDEX NAME)

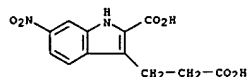
L14 ANSWER 6 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



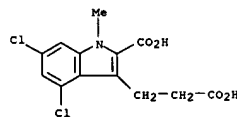
RN 132004-35-4 HCAPLUS
CN 1H-Indole-3-propanoic acid, 2-carboxy-4-nitro- (9CI) (CA INDEX NAME)



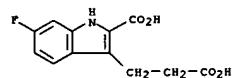
RN 132004-36-5 HCAPLUS
CN 1H-Indole-3-propanoic acid, 2-carboxy-6-nitro- (9CI) (CA INDEX NAME)



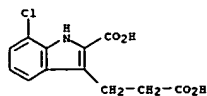
RN 139896-76-7 HCAPLUS
CN 1H-Indole-3-propanoic acid, 2-carboxy-4,6-dichloro-1-methyl- (9CI) (CA INDEX NAME)



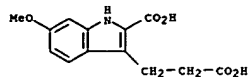
RN 139896-77-8 HCAPLUS
CN 1H-Indole-3-propanoic acid, 2-carboxy-6-fluoro- (9CI) (CA INDEX NAME)



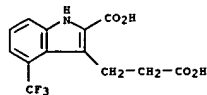
L14 ANSWER 6 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



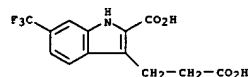
RN 132004-30-9 HCAPLUS
CN 1H-Indole-3-propanoic acid, 2-carboxy-6-methoxy- (9CI) (CA INDEX NAME)



RN 132004-32-1 HCAPLUS
CN 1H-Indole-3-propanoic acid, 2-carboxy-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



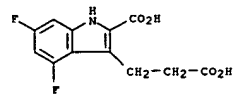
RN 132004-33-2 HCAPLUS
CN 1H-Indole-3-propanoic acid, 2-carboxy-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)



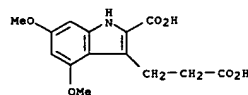
RN 132004-34-3 HCAPLUS
CN 1H-Indole-3-propanoic acid, 2-carboxy-4-fluoro- (9CI) (CA INDEX NAME)

L14 ANSWER 6 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

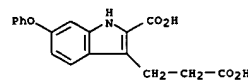
RN 139896-78-9 HCAPLUS
CN 1H-Indole-3-propanoic acid, 2-carboxy-4,6-difluoro- (9CI) (CA INDEX NAME)



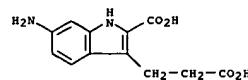
RN 139896-79-0 HCAPLUS
CN 1H-Indole-3-propanoic acid, 2-carboxy-4,6-dimethoxy- (9CI) (CA INDEX NAME)



RN 139896-80-3 HCAPLUS
CN 1H-Indole-3-propanoic acid, 2-carboxy-6-phenoxy- (9CI) (CA INDEX NAME)

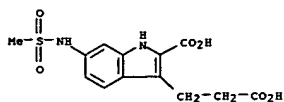


RN 139896-81-4 HCAPLUS
CN 1H-Indole-3-propanoic acid, 6-amino-2-carboxy- (9CI) (CA INDEX NAME)

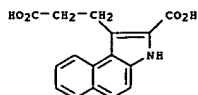


RN 139896-82-5 HCAPLUS
CN 1H-Indole-3-propanoic acid, 2-carboxy-6-[(methylsulfonyl)amino]- (9CI) (CA INDEX NAME)

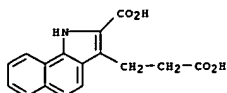
L14 ANSWER 6 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



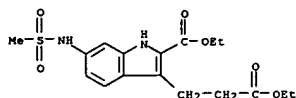
RN 139896-83-6 HCAPLUS
CN 3H-Benz[e]indole-1-propanoic acid, 2-carboxy- (9CI) (CA INDEX NAME)



RN 139896-84-7 HCAPLUS
CN 1H-Benz[g]indole-3-propanoic acid, 2-carboxy- (9CI) (CA INDEX NAME)

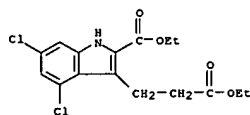


IT 139896-90-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
[preparation and hydrolysis and mesylation of]
RN 139896-90-5 HCAPLUS
CN 1H-Indole-3-propanoic acid, 2-(ethoxycarbonyl)-6-[(methylsulfonyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

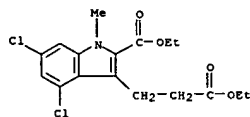


IT 139896-98-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
[preparation and hydrolysis and reduction of]

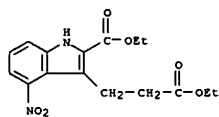
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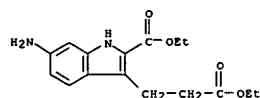
RN 139896-86-9 HCAPLUS
CN 1H-Indole-3-propanoic acid, 4,6-dichloro-2-(ethoxycarbonyl)-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 139896-87-0 HCAPLUS
CN 1H-Indole-3-propanoic acid, 2-(ethoxycarbonyl)-4-nitro-, ethyl ester (9CI) (CA INDEX NAME)

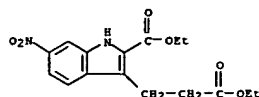


RN 139896-89-2 HCAPLUS
CN 1H-Indole-3-propanoic acid, 6-amino-2-(ethoxycarbonyl)-, ethyl ester (9CI) (CA INDEX NAME)

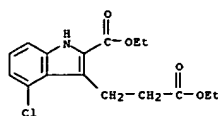


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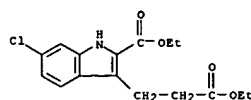
RN 139896-88-1 HCAPLUS
CN 1H-Indole-3-propanoic acid, 2-(ethoxycarbonyl)-6-nitro-, ethyl ester (9CI) (CA INDEX NAME)



IT 130798-57-1P 130798-58-2P 130828-27-5P
139896-86-9P 139896-87-0P 139896-89-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
[preparation and hydrolysis of]
RN 130798-57-1 HCAPLUS
CN 1H-Indole-3-propanoic acid, 4-chloro-2-(ethoxycarbonyl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 130798-58-2 HCAPLUS
CN 1H-Indole-3-propanoic acid, 6-chloro-2-(ethoxycarbonyl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 130829-27-5 HCAPLUS
CN 1H-Indole-3-propanoic acid, 4,6-dichloro-2-(ethoxycarbonyl)-, ethyl ester (9CI) (CA INDEX NAME)

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ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA issue.
AB The title compds. (I) have broad-spectrum antibacterial activities. A stream of EtNH2 was introduced with mech. stirring into 98.5 g. MeCOCH2CO2Et for 3 hrs. at 35-40° to give 104 g. R2C(NHRI):CHCO2Et (II, R1 = Et, R2 = Me) (IIa), b20 116-18°, n25D 1.4941. The following II were similarly prepared (R1 and R2 given): Pr, Me, b14 119-19.5°; iso-Pr, Me, b11 106-6.5°; Bu, Me, b14 129.5-31.0°; CH2CH2OH, Me, and Et, Et, b14 118-21°. A solution of 122 g. IIa in 60 ml. Me2CO was thoroughly swept with N, treated with 10.9 g. toluquinone, heated 2 hrs. on the steam bath, and cooled to give III (R1 = Et, R2 = Me, R3 = CO2Et, R4 = H, R5 = OH, R6 = Me, R7 = H) (IIIa), m. 196-8° (aqueous EtOH). The following III were similarly prepared (R3 = CO2Et, R6 = OH, R7 = H; R1, R2, R6, and m.p. given): Me, Me, Me, 222-5°; Pr, Me, Me, 193.5-5.0°; iso-Pr, Me, Me, 202-3°; Bu, Me, Me, 176-7°; CH2CH2OH, Me, Me, 190.6-7.5°; Et, Et, Me, 164-6°; Et, Me, Et, 207-8°. A stirred mixture of 50 g. IIIa and 500 ml. 20% HCl was refluxed 2 hrs. and worked up in the usual manner to give III (R1 = Et, R2 = Me, R3 = H, R4 = H, R5 = OH, R6 = Me, R7 = H) (IIIb), m. 113-17° (CH2Cl2-petr. ether b.p. 30-60°) and m. 90-2° (direct from mother liquor). The following III were similarly prepared (R3 = R4 = H, R5 = OH, and R7 = H; R1, R2, R6, and m.p. given): Me, Me, Me, 130-1.5°; Pr, Me, Me, 125-8°; iso-Pr, Me, Me, 94-5°; Bu, Me, Me, 73.5-5.0°; CH2CH2OH, Me, Me, 121-3°; Et, Et, Me, 88-90°; Et, Me, Et, 80.5-1.5°. A stirred solution of 49.1 g. IIIb in 300 ml. EtOH and 600 ml. 2N NaOH solution was treated dropwise during 1.5 hrs. at reflux under N with 100 g. Me2SO4, the mixture refluxed 1 hr. and extracted with EtOAc, and the extract worked up to give III (R1 = Et, R2 = Me, R3 = H, R4 = H, R5 = MeO, R6 = Me, R7 = H) (IIIc), m. 56-7° (hexane). The following III were similarly prepared (R3 = R4 = H, R5 = MeO, R7 = H; R1, R2, R6, phys. state, and m.p. given): H, Me, Me, solid, 94-6°; Me, Me, Me, solid, 75-7°; Pr, Me, Me, oil, --; iso-Pr, Me, Me, oil, --; Bu, Me, Me, oil, --; CH2CH2OH, Me, Me (IIId), solid, 78-80°; Et, Et, Me, oil, --; and Et, Me, Et, oil, --. An ice-chilled, stirred solution of 12.7 g. IIId in 100 ml. C6H6 was treated dropwise with 10 ml. MeSO2Cl and kept at 0° to 5° 15 hrs. to give III (R1 = CH2CH2OSO2Me, R2 = Me, R3 = H, R4 = H, R5 = MeO, R6 = Me, R7 = H), m. 118-20° (decomposition). A stirred suspension of 16.7 g. 2,5-dimethyl-4-nitrophenol in 50 ml. H2O at 40-5° was treated alternately and in portions with a solution of 7.0 g. NaOH in 18 ml. H2O and 12 ml. Me2SO4 and kept 2 hrs. at room temperature to give 2,5-dimethyl-4-nitroanisole (IV), m. 90-2° (aqueous MeOH). EtOH (6.25 ml.) was added to a stirred slurry of 2.15 g. K in C6H6, the C6H6 distilled, 50 ml. C6H6 added and again removed, and a slurry of the residue in 100 ml. Et2O treated with 7.3 g. (CO2-Et)2 and then with 9.05 g. IV in 150 ml. Et2O and stirred 18 hrs. at room temperature to give 6.123 g. 5-methoxy-4-methyl-2-nitrophenyl-pyruvic acid (V), m. 167-70°. A solution of 42.0 g. V in 230 ml. 17% NH4OH and 115 ml. H2O was treated with a hot solution of FeSO4.7H2O in 340 ml. H2O and the mixture stirred 1 hr. on the steam bath to give III (R1 = H, R2 = CO2H, R3 = H, R4 = H, R5 = MeO, R6 = Me, R7 = H) (IIIf), m. 240-2° (gas evolution) (dilute AcOH). A solution of 4.0 g. IIIf in 100 ml. methanolic HCl was refluxed 16 hrs. to give III (R1 = H, R2 = CO2Me, R3 = H, R4 = H, R5 = MeO, R6 = Me, R7 = H) (IIIf), m. 147-9° (dilute MeOH). A stirred solution of 15.4 g. IIIf in 500 ml. C6H6 was treated with 3.55 g. of a 50.7% suspension of NaH in mineral oil. The mixture was refluxed 45 min. and then treated with 25 ml. Et2SO4 during 15 min. and refluxed 4 hrs. to give III (R1 = Et, R2 = CO2Et, R3 = H, R4 = H, R5 = MeO, R6 = Me, R7 = H). (IIIf), m. 101-2°. A mixture of 7.0 g. IIIf and 2.17 g. LiAlH4 in 470 ml. Et2O was refluxed 2.5 hrs., stirred 16 hrs. at room temperature, and worked up in the usual manner to give III (R1 = Et, R2 = CH2OH, R3 = H, R4 = H, R5 = MeO, R6 = Me, R7 = H) (IIIf), m.

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 103-6° (30-60° petr. ether). A soln. of 5.49 g. IiIh and 7 ml. Ac2O in 60 ml. C5H5N was kept 17 hrs. at room temp. to give III (R1 = Et, R2 = CH2OAc, R3 = H, R4 = H, R5 = MeO, R6 = Me, R7 = H), m. 96-7°. To stirred, ice-chilled HCONMe2 (VII) (200 ml.) was added dropwise at 0° to 5° 55 g. POC13 and with a soln. of 66.35 g. IiIc in 150 ml. VII at 5° to give 70.5g. IiI (R1 = Et, R2 = Me, R3 = CHO, R4 = H, R5 = MeO, R6 = Me, R7 = H) (IiIi), m. 134-6°. The following IiI were similarly prepd. (R3 = CHO, R4 = H, R5 = MeO, and R7 = H; R1, R2, R6, and m.p. given): H, Me, Me, 227-8.5°; Me, Me, Me, 174-8°; Pr, Me, Me, 117.5-9.5°; iso-Pr, Me, Me, Me, 172-4°; Bu, Me, Me, 96-7°; Et, Et, Me, 95.5-7.0°; Et, Me, Et, 109-10°; CH2CH2OSO2Me, Me, Me, 187.5-9.0° (decompn.); Et, CH2OAc, Me, 122.5-3.5°; and Et, CO2Me, Me (IiIin), 178.5-80.0°. A stirred mixt. of 12.9 g. IiIc, 10 g. AcONa, and 300 ml. Ac2O was refluxed 6 hrs. to give IiI (R1 = Et, R2 = Me, R3 = H, R5 = MeO, R6 = Me, R7 = H) (IiIj), m. 88-9°. A mixt. of 38.4 g. IiIi and 46.0 g. AlCl3 in 1 l. xylene was refluxed 5 hrs. with stirring, cooled, and poured onto cracked ice to give IiI (R1 = Et, R2 = Me, R3 = CHO, R4 = H, R5 = OH, R6 = Me, R7 = H), m. 256-9° (decompn.) (Me2CO). IiIj similarly gave IiI (R1 = Et, R2 = Me, R3 = Ac, R4 = H, R5 = OH, R6 = Me, R7 = H), m. 262-5° (decompn.) (Me2CO). To a stirred soln. of 18.0 g. K nitridisulfonate (VIII) in 400 ml. H2O and 200 ml. M/6 KH2PO4 was added a soln. of 2.47 g. IiIa in 500 ml. Me2CO and the mixt. kept 16 hrs. at room temp. and worked up to give IX (R1 = Et, R2 = Me, R3 = CO2Et, R6 = Me, R7 = H) (IXa), m. 115-18°. The following IX were similarly prepd. from the corresponding 5-hydroxyindole derivs. (R1, R2, R3, R6, R7, and m.p. given): Et, Me, CHO, Me, H (IXb), 214-16° (Me2CO-hexane); and Et, Me, Ac, Me, H, 164-6° (CH2Cl2-petr. ether, b. 30-60°). A soln. of 400 mg. IXa in 6 ml. AcOH was treated with 0.125 ml. BF3-etherate and the mixt. kept 1 hr. at room temp. and poured onto cracked ice to give 450 mg. IiI (R1 = Et, R2 = Me, R3 = CO2Et, R4 = OAc, R5 = OAc, R6 = Me, R7 = OAc) (IiIk), m. 157-9°. The following IiI were similarly prepd. (R1, R2, R3, R4, R5, R6, R7, and m.p. given): Et, Me, CHO, OAc, OAc, Me, OAc, 194-5°; and Et, Me, Ac, OAc, OAc, Me, OAc, --. A stirred mixt. of 2.25 g. IiIi in 100 ml. H2O and 20 ml. 20% NaOH soln. was refluxed 30 min. under N and filtered and the filtrate treated with a stream of air 30 min., acidified with concd. HCl, and extd. with CH2Cl2 to give I (R1 = Et, R2 = Me, R3 = CO2H, R5 = OH, R6 = Me) (Ia), m. 220-3° (CH2Cl2-petr. ether, 30-60°). A stirred mixt. of 691 mg. Ia, 5.5 g. K2CO3, and 11 ml. Me2SO4 in 250 ml. Me2CO was refluxed 45 min. and stirred 2 hrs. at room temp. to give I (R1 = Et, R2 = Me, R3 = CO2Me, R5 = MeO, R6 = Me) (Ic), m. 82-3° (dil. Me2CO). A mixt. of 1.0 g. Ib (see below) in tetrahydrofuran was refluxed 13 hrs., distd. to dryness, and treated with 4 ml. MeOH to give I (R1 = Et, R2 = Me, R3 = CHO, R5 = EtO, R6 = Me), m. 117-19°. A stirred soln. of 334 mg. Ic in 25 ml. tetrahydrofuran was treated with 197 mg. LiAlH4 to give I (R1 = Et, R2 = Me, R3 = CH2OH, R5 = MeO, R6 = Me), m. 85-7°. A stirred soln. of 500 mg. Id (see below) in 150 ml. MeOH was swept with a stream of N, heated to reflux, and treated with 500 mg. NaBH4 to give I (R1 = Et, R2 = Me, R3 = CH2OH, R5 = MeO, R6 = Me) (Ie), m. 85.5-6.5° (CH2Cl2-petr. ether). The following I were similarly prepd. by the various procedures given above: (R1, R2, R3, R5, R6, and m.p. given): Et, Me, CHO, OH, Me (Ib), 213-19°; Et, Me, Ac, OH, Me, 172-5°; Et, Me, CHO, MeO, Me (Id), 133-5°; Et, Me, Ac, MeO, Me, 126-7°; Et, Me, CH2OH, Me, 65-70°; and Et, Me, CH2CH2OH, MeO, Me, --. IiIe (3.61 g.) was heated at 260-70° until the melt became quiescent, was held briefly at 300°, cooled, and dissolved in Et2O, and the soln. washed with Na2CO3 soln. to give 2.12 g.

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 with the appropriate nucleophile (R2 = Me, R3 = CHO, R4 = NH2, R5 = MeO, R6 = Me, R7 = H; R1 and m.p. given): CH2CH2SCN, 190-3°; CH2CH2Cl, 120-3°; and CH2CH2SMe, 128.5-30°. A soln. of 2.466 g. IiIi in 100 ml. MeOH contg. 6 ml. 10% K2CO3 was stirred 1 hr. at room temp. under N, acidified with 45 ml. AcOH, and worked up to give IiI (R1 = CH2CH2OH, R2 = Me, R3 = CHO, R4 = NH2, R5 = MeO, R6 = Me, R7 = H), m. 157-9°. A soln. of 5.38 g. IiIi in 1 l. Me2O was added to a stirred soln. of 25 g. VIII and treated as described above to give I (R1 = R2 = Me, R3 = CHO, R5 = MeO, R6 = Me, m. 146-8°). The following I were similarly prepd. (R3 = CHO, R5 = MeO; R1, R2, R6, and m.p. given): H, Me, Me, 236-40°; Et, Me, Me (Ij), 125-9°; Pr, Me, Me, 134-5°; iso-Pr, Me, Me, 97-9°; Bu, Me, Me, 82.5-83°; Et, Et, Me, 76.07-5°; Et, Me, Et, 81.0-3.5°; CH2CH2OSO2Me, Me, Me, 143-4°; Et, CH2OAc, Me, 142-4°; Et, CH2OH, Me (Ie), 128.5-30.0°; CH2CH2F, Me, Me, 114-17°; CH2CH2NH3, Me, Me, 80-1°; CH2CH2SCN, Me, Me, --; CH2CH2Cl, Me, Me, 113.0-13.5°; CH2CH2SMe, Me, Me, 77-9°; CH2CH2OH, Me, Me, 129-31°; and Et, CONH2, Me, 197-9°. A soln. of 226 mg. Ie, 10 mg. p-MeC6H4SO3H, H2O, and 92 mg. dihydropyran in 30 ml. C6H6 was stirred 3 hrs. at room temp. to give I (R1 = Et, R2 = tetrahydropyranyloxymethyl, R3 = CHO, R5 = MeO, R6 = Me). The following I were prepd. according to the procedures given above (R1, R2, R3, R5, R6, and m.p. given): tetrahydropyranyloxymethyl, Me, CHO, MeO, Me, --; Et, CO2H, CHO, OH, Me, 161-3°; and Et, CO2Me, CHO, MeO, Me (If), --. The following IiI was also prepd. from the appropriate compd. with Ac2O-BF3 etherate, R1 = Et, R2 = CO2Me, R3 = diacetoxyethyl, R4 = AcO, R5 = AcO, R6 = Me, R7 = AcO), m. 139-49°. A mixt. of 532 mg. IiIi and 105 mg. 10% Pd-C in 100 ml. EtOH contg. 1 ml. H2O was shaken under H 1.75 hrs., filtered, and added with stirring to a soln. of 5.06 g. VIII to give I (R1 = Et, R2 = H, R3 = CH2OH, R5 = MeO, R6 = Me), m. 78-81° (Et2O-petr. ether, b. 30-60°). The following I were similarly prepd. according to the procedures given above (R3 = CH2OH, and R5 = MeO; R1, R2, R6, and m.p. given): Et, Me, Me, 85-7°; Et, CO2Me, Me, 80-2°; H, Me, Me, 233-5°; Me, Me, --; Pr, Me, Me, --; iso-Pr, Me, Me, 76-8°; Bu, Me, Me, 68-70°; Et, Et, Me, --; Et, Me, Et, 128-9°; Et, tetrahydropyranyloxymethyl, Me, --; CH2CH2F, Me, Me, 116-18°; CH2CH2NH3, Me, Me, --; CH2CH2SCN, Me, Me, --; CH2CH2Cl, Me, Me, --; CH2CH2SMe, Me, Me, --; Et, CO2Me, Me, 83-4°; and Et, CONH2, Me, 202-2°. If and Ifa were treated as above to give I (R1 = Et, R2 = CO2Me, R3 = CH2OH, R5 = MeO, R6 = Me), m. 82-4°. A mixt. of 33 g. 2-acetyl-1,3-cyclohexanedione, 20 g. EtNH2, and 135 ml. MeOH was heated 12 hrs. at 150° in a steel bomb to give 1-ethyl-4,5,6,7-tetrahydro-2-methyl-4-oxoindole (XI), m. 74-5° (cyclohexane). Similarly, 2-acetyl-5-methyl-1,3-cyclohexanedione gave 2,6-dimethyl-1-ethyl-4,5,6,7-tetrahydro-4-oxoindole (XI), m. 77-9°. A mixt. of 10.5 g. X, 2.5 g. 10% Pd-C, and 50 ml. cumene was refluxed 3 hrs. to give Et (R1 = Et, R2 = Me, R3 = H, R4 = OH, R5 = R6 = R7 = H) (IiIj), m. 98-102°. Similarly XI gave IiI (R1 = Et, R2 = Me, R3 = H, R4 = OH, R5 = H, R6 = Me, R7 = H), m. 141-3°. An ice-cooled suspension of 64 g. MeONa in 600 ml. C6H6 was treated with 88.8 g. HCO2Et and 65.7 g. XI in 600 ml. C6H6 and the mixt. stirred overnight at room temp., cooled in an ice bath, and treated with 1200 ml. 5% NaOH to give 70.2 g. 2,6-dimethyl-1-ethyl-5-hydroxymethylene-4,5,6,7-tetrahydro-4-oxoindole (XI), m. 71-4° (petr. ether). A soln. of 4.51 g. XII in 30 ml. dioxane was stirred with 4.54 g. dichlorodicyanobenzoquinone in 30 ml. dioxane to give IiI (R1 = Et, R2 = Me, R3 = H, R4 = OH, R5 = CHO, R6 = Me, R7 = H) (IiIj), m. 129-30.5° (hexane). A soln. of 1.09 g. IiIy in EtOH was treated with 1.0 g. 10% Pd-C and shaken with H in a Parr app. to give IiI (R1 = Et, R2 = Me, R3 = H, R4 = OH, R5 = Me, R6 = Me, R7 = H), m. 98-102° (hexane). A soln. of 4.0 g. IiIix in 75 ml. H2O contg. 1.35 g. NaOH was treated with 3.4 g. Ac2O and 3.0 g. AcONa to give IiI (R1 = Et, R2 = Me, R3 = H, R4 = OAc, R5 = R6 = R7 = H) (IiIiz), m.

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 IiI (R1 = R2 = R3 = R4 = H, R5 = MeO, R6 = Me, R7 = H), m. 119-20°, which was treated as above with POC13 to give IiI (R1 = R2 = H, R3 = CHO, R4 = H, R5 = MeO, R6 = Me, R7 = H) (IiIi), m. 192-5°. A mixt. of 1.75 g. IiIi and 30 ml. 40% KOH was heated with stirring on the steam bath and treated with 10 g. Et2SO4 during 1 hr. to give IiI (R1 = Et, R2 = H, R3 = CHO, R4 = H, R5 = MeO, R6 = Me, R7 = H) (IiIia), m. 92-4°. A stirred soln. of 1.085 g. IiIa in 12 ml. concd. H2SO4 was treated dropwise during 30 min. with 0.425 g. NaNO3 in 7 ml. concd. H2SO4 and the mixt. stirred 45 min. and poured onto ice-H2O to give IiI (R1 = Et, R2 = H, R3 = CHO, R4 = NO2, R5 = MeO, R6 = Me, R7 = H) (IiIib), m. 150-2° (Me2CO-hexane). Similarly prepd. was IiI (R1 = Et, R2 = Me, R3 = CHO, R4 = NO2, R5 = MeO, R6 = Me, R7 = H), m. 155-7°. A stirred soln. of 10 g. IiIa in 300 ml. AcOH was treated dropwise with 10 ml. yellow fuming HNO3 and the mixt. stirred 1 hr. and treated with H2O to give IiI (R1 = Et, R2 = CO2Me, R3 = CHO, R4 = NO2, R5 = MeO, R6 = Me, R7 = H) (IiIic), m. 182-4° (Me2CO-hexane), and a filtrate which yielded IX (R1 = Et, R2 = CO2Et, R3 = CHO, R6 = Me, R7 = H), m. 207-10° (Me2CO-hexane). The following IiI were prepd. by the procedures given above (R3 = CHO, R4 = NO2, R6 = MeO, and R7 = H; R1, R2, R6, and m.p. given): H, Me, Me, 280°; Me, Me, Me (IiIir), 183-7°; Pr, Me, Me, 136-8°; iso-Pr, Me, Me, --; Bu, Me, Me, 127-8°; Et, Et, Me, 151-4°; Et, Me, Et, 181.0-2.5°; CH2CH2OSO2Me, Me, Me (IiIip), 181.5-3.0°; and Et, CH2OAc, Me, 198-200°. A stirred mixt. of 8.0 g. IiIa and 250 ml. 5% NaOH soln. was refluxed, cooled, and acidified with concd. HCl to give IiI (R1 = Et, R2 = CO2H, R3 = CHO, R4 = NO2, R5 = MeO, R6 = Me, R7 = H) (IiIiq), m. 216-17° (Me2CO). An ice-chilled stirred soln. of 2.154 g. IiIq and 1.14 ml. Et3N in 60 ml. VII was treated dropwise with 0.79 ml. ClCO2Et at 0-5°. NH3 gas was then passed through the mixt. for 10 min. to give IiI (R1 = Et, R2 = CONH2, R3 = CHO, R4 = NO2, R5 = MeO, R6 = Me, R7 = H), m. 252-4° (Me2CO). A mixt. of 5.0 g. IiIp and 5.0 g. powd. KF, 2H2O in 160 ml. MeOH was heated in a stainless steel bomb at 150° 18 hrs. and worked up to give IiI (R1 = CH2CH2F, R2 = Me, R3 = CHO, R4 = NO2, R5 = MeO, R6 = Me, R7 = H), m. 175-80° (Me2CO-petr. ether, b. 60-70°). A mixt. of 500 mg. IiIp and 1.0 g. AcONa in 25 ml. VII was heated 15 hrs. on the steam bath, cooled, and dild. with H2O to give IiI (R1 = CH2CH2OAc, R2 = Me, R3 = CHO, R4 = NO2, R5 = MeO, R6 = Me, R7 = H), m. 179-80°. A stirred soln. of 13.15 g. IiIir in 875 ml. EtOH and 375 ml. H2O was heated on the steam bath and treated with a soln. of FeSO4.7H2O in 1250 ml. H2O and the mixt. heated to boiling and at 30-60 sec. intervals treated with 10 ml. concd. NH4OH until 150 ml. were added to give IiI (R1 = R2 = Me, R3 = CHO, R4 = NH2, R5 = MeO, R6 = Me, R7 = H) (IiIiu), m. 150-4°. The following IiI were similarly prepd. by this procedure (R3 = CHO, R4 = NH2, R5 = MeO, R7 = H; R1, R2, R6, and m.p. given): Et, Me, Me, 117.5-18.5°; Et, Et, Me, --; Pr, Me, Me, 128-9°; Bu, Me, Me, 129.5-31.0°; Et, CH2OH, Me, 182.0-2.5°; Et, CH2OAc, Me, 136-8°; and Et, CONH2, Me, 202-3°. A stirred soln. of 15.0 g. IiIip in 450 ml. AcOH and 45 ml. H2O was heated on the steam bath and treated with 20.0 g. Fe filings during 2 hrs. to give IiI (R1 = CH2CH2OSO2Me, R2 = Me, R3 = CHO, R4 = NH2, R5 = MeO, R6 = Me, R7 = H) (IiIis), m. 133-5°. The following IiI were similarly prepd. by this procedure (R3 = CHO, R4 = NH2, R5 = MeO, R7 = H; R1, R2, R6, and m.p. given): H, Me, Me, --; iso-Pr, Me, Me, --; Et, Me, Et, 110.5-12.5°; CH2CH2F, Me, Me, 139-41°; and CH2CH2OAc, Me, Me (IiIit), 178-80°. A mixt. of 300 mg. IiIs and 300 mg. NaN3 in 10 ml. VII was refluxed 16 hrs. and poured into 150 ml. H2O to give IiI (R1 = CH2CH2NH3, R2 = Me, R3 = CHO, R4 = NH2, R5 = MeO, R6 = Me, R7 = H), m. 123-4°. The following IiI were similarly prepd. by treating IiIs

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 71-3°. The following IiI were similarly prepd. (R1, R2, R3, R4, R5, R6, R7, and m.p. given): Et, Me, H, OAc, H, Me, H, 61-3°; and Et, Me, H, OAc, Me, Me, H, 113-14.5°. An ice-cooled mixt. of 2.0 g. POC13 and 15 ml. VII was treated dropwise with 3.02 g. IiIi in 15 ml. VII and the mixt. stirred 90 min. and poured onto a mixt. of ice and 10% Na2CO3 to give IiI (R1 = Et, R2 = Me, R3 = CHO, R4 = OAc, R5 = R6 = R7 = H) (IiIias), m. 165-8° (MeOH). A mixt. of 3.14 g. IiIias, 20 ml. MeOH, and 60 ml. 5% NaOH was dild. with 200 ml. MeOH and carefully neutralized with AcOH to give IiI (R1 = Et, R2 = Me, R3 = CHO, R4 = OH, R5 = R6 = R7 = H) (IiIibb), m. 169-70° (MeOH). The following IiI derivs. were similarly prepd. by the above procedures (R1, R2, R3, R4, R5, R6, R7, and m.p. given): Et, Me, CHO, OAc, H, Me, H, 168-71°; Et, Me, CHO, OAc, Me, Me, H, 165-8°; Et, Me, CHO, OH, H, Me, H, 178-80°; and Et, Me, CHO, OH, Me, Me, H, 162-3.5°. To a stirred soln. of 1.98 g. VIII in 180 ml. M/18 KH2PO4 was added a hot soln. of 375 mg. IiIibb in 50 ml. Me2CO and worked up as described above to give I (R1 = Et, R2 = Me, R3 = CHO, R5 = R6 = H) (Ij), m. 148-55°. The following I were similarly prepd. by this procedure (R1, R2, R3, R5, R6, and m.p. given): Et, Me, CHO, H, Me, 146-9°; Et, Me, CHO, Me, Me, 122-7°; and Et, Me, H, H, H (Ih), 86-7°. An ice-cooled mixt. of 1.13 g. Ih, 1.1 g. Zn dust, 10 ml. Ac2O, and 0.5 ml. C5H5N was kept 30 min. at room temp. to give IiI (R1 = Et, R2 = Me, R3 = H, R4 = OAc, R5 = R6 = H, R7 = OAc) (IiIicc). IiIicc was treated with POC13 as above to give IiI (R1 = Et, R2 = Me, R3 = CHO, R4 = OAc, R5 = R6 = H, R7 = OAc) (IiIidd), m. 124-6° (MeOH). IiIidd was treated with FeCl3.6H2O to give I (R1 = Et, R2 = Me, R3 = CHO, R5 = R6 = H), m. 148-59°.

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 REENTER FILE 'HCAPLUS'
 AND TRY AGAIN, OR ENTER '?' FOR MORE INFORMATION.

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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

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